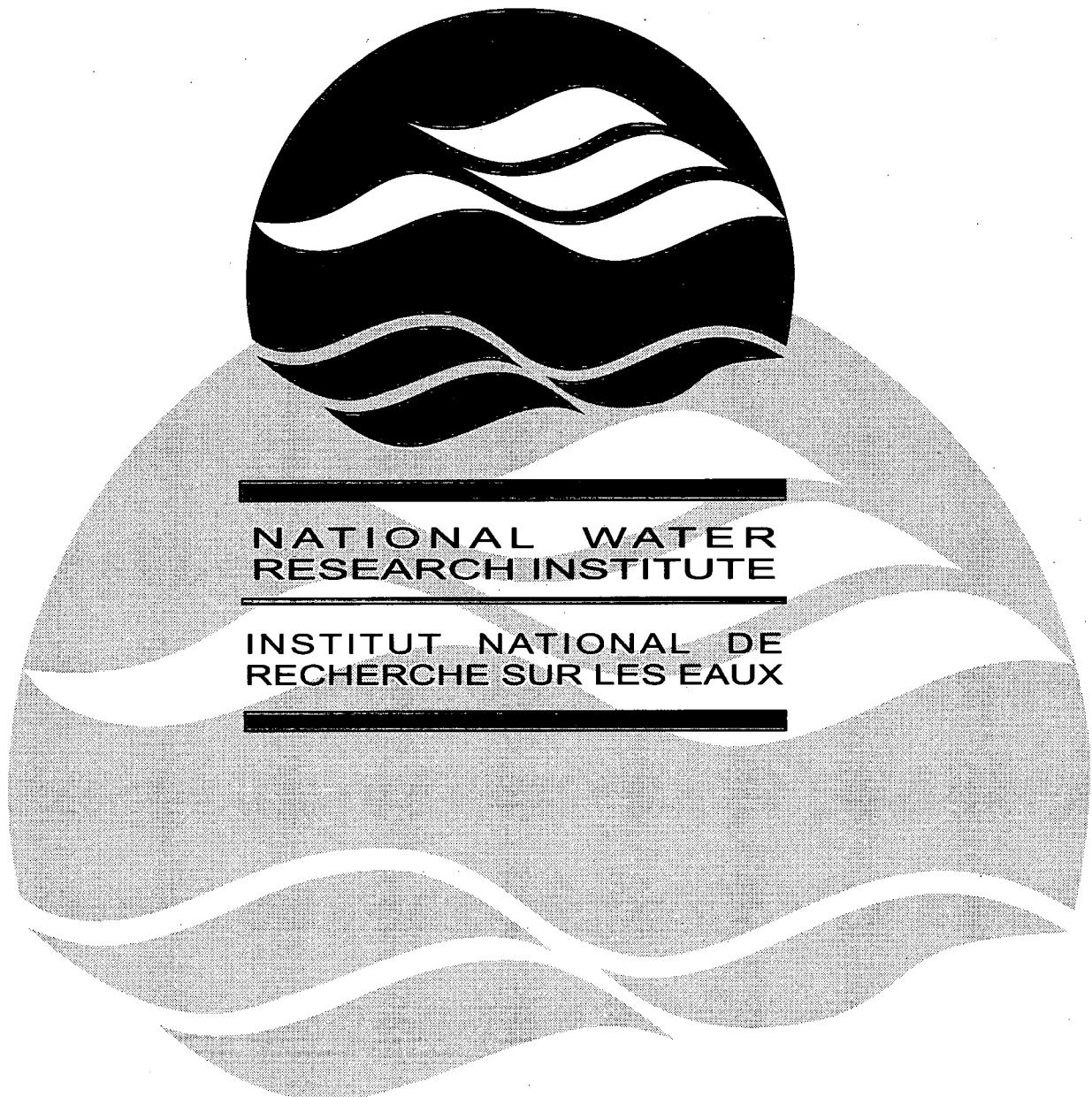


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**PROBABILISTIC NEURAL NETWORK (PNN)  
METHODOLOGY FOR THE PREDICTION OF  
ACUTE TOXICITY OF CHEMICALS TO FATHEAD  
MINNOW BASED SOLELY ON CHEMICAL  
STRUCTURE-DERIVED INPUT PARAMETERS**

Kaiser, K.L.E. and S.P. Niculescu

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STRUCTURE-DERIVED INPUT PARAMETERS**

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NWRI Cont. #99-01

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## **Management Perspective**

This report, prepared in partial fulfilment of a collaborative research arrangement with CCEB, provides a brief overview of the methodology, its advantages and limitations. In addition, it gives a full description of the used input and derived output values for the training set of chemicals.

This methodology has been applied to approximately 700 chemicals, as provided by CCEB, for the prediction of acute toxic effects to fathead minnow (*Pimephales promelas*). These data are contained in Appendix 2 of this report and will be compared, under a separate contract, let and supervised directly by CCEB, with measured toxicity data and estimates derived from other programs in use by CCEB, including Ecosar and Topkat.

## **Sommaire à l'Intention de la Direction**

Ce rapport, qui présente les résultats d'une étude s'inscrivant dans un projet de recherche conjoint avec la DEPCC, donne un bref aperçu de la méthode, de ses avantages et de ses limites. De plus, il décrit de façon détaillée les valeurs d'entrée utilisées et les valeurs de sortie dérivées pour l'ensemble de produits chimiques d'apprentissage.

Cette méthode a été appliquée à environ 700 produits chimiques, fournis par la DEPCC, en vue de la prévision de leurs effets toxiques aigus sur la tête-de-boule (*Pimephales promelas*). Les données sont présentées à l'Annexe 2 du présent rapport et seront comparées, dans le cadre d'un contrat distinct accordé et supervisé directement par la DEPCC, avec des données de toxicité mesurée et des estimations issues d'autres programmes utilisés par la DEPCC, dont Ecosar et Topkat.

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## **Abstract**

This report gives an overview of the probabilistic neural network methodology, the individual results, and a brief comparison with other available toxicity estimation models for the prediction of 96-hr LC50 values for the fathead minnow (*Pimephales promelas*) based on an 865 chemicals data set. It has been prepared as a background report for the Commercial Chemicals Evaluation Branch, Environment Canada, Ottawa.

## **Résumé**

Ce rapport présente un aperçu de la méthode du réseau neuronal probabiliste, les résultats individuels et une brève comparaison avec d'autres modèles d'estimation de la toxicité pour la prévision des CL50 sur 96 heures pour la tête-de-boule (*Pimephales promelas*), à partir d'un ensemble de données portant sur 865 produits chimiques. Il a été préparé à titre de rapport d'information pour la Direction de l'évaluation des produits chimiques commerciaux d'Environnement Canada.

## **Introduction**

There is a rising interest in developing useful models which allow the prediction of toxicological effects and concentrations of chemicals. Traditional methods in Quantitative Structure-Activity Relationships (QSARs) are based on comparatively small sets of chemicals with relatively small, easily described variations in substituents. In contrast, the applied environmental field deals with a broad spectrum of substances arising from many sources. For example, the Canadian Domestic Substances and Non-Domestic Substances Lists of substances in commerce include over 66,000 compounds. The OECD list of High Production Volume Chemicals contains over 4,000 substances. Given the present rate of approximately 3 million compounds being added annually to the Chemical Abstracts Service registration number index, the number of compounds in commerce is likely to grow at a significant rate as well. For many of these substances, very little or no toxicological information is available and their fate and effects in the environment are unknown. As these substances encompass all kinds of materials, traditional QSAR methods to estimate their toxicities are generally not applicable because these are limited to well defined congeneric sets (for example, Nendza and Russom, 1991). Therefore, different methods need to be explored for the simultaneous modelling and prediction of the effects of a great variety of structures. Neural networks have recently gained much attention and initial applications have proven very promising (Devillers, 1996a, 1996b).

Our earlier investigations of the applicability and usefulness of neural networks include: the comparative study of linear regression and probabilistic neural network (PNN) methods for fathead minnow and *Vibrio fischeri* bacteria toxicity data (Kaiser and Niculescu 1998a, 1998b; Kaiser, Niculescu and McKinnon 1997; Kaiser, Niculescu and Schüürmann 1997), the use of feed forward backpropagation neural networks for fathead minnow toxicity data and the influence of data pre-processing and kernel selection on the quality of the predictions of PNN predictions for both fathead minnow and *Vibrio fischeri* toxicity data (Kaiser, Niculescu and Schüürmann 1997; Niculescu, Kaiser et Schüürmann 1998).

We describe here details on the application of our recently developed methodology (Kaiser and Niculescu, 1998a) for the prediction of the acute 96-hr LC50 to the fathead minnow (*Pimephales promelas*) based on PNNs. In contrast to most other toxicological models, the octanol/water partition coefficient is not used as input parameter. The information fed into the neural network is solely based on simple molecular descriptors as can be derived from the chemicals' structures. The present work builds on the results obtained from our earlier investigations which were designed to determine certain basic principles and comparisons of model types.

## Probabilistic Neural Networks: A brief overview

The PNNs are the result of the interdisciplinary research between the field of Bayesian Statistics and Artificial Intelligence. The fundamental idea behind the use of PNNs as Bayesian predictor systems is simple, elegant, and has a very solid mathematical foundation. The predictions are computed based on the Bayesian estimate of the multivariate probability density function of the network's output vector of values conditional with respect to the data used for training. Meisel (1972) developed the theory behind the statistical methodology. The limited resources offered by the computers available at that time were completely inappropriate to handle the huge volume of mathematical operations required by the algorithm. The real progress in implementing it was realized by Specht's (1990) who discovered the fact that the statistical mathematical algorithm can be split up into a large number of simple sub-processes, which are separate procedures on their own, and most of which can be run in parallel. These are the characteristics of a neural network, and Specht created it.

The architecture of the PNNs used by our methodology of predicting toxicity values to the fathead minnow is presented in Figure 1 and involves four neuron layers. The input layer is the gateway through which we feed input information into the network. It contains a neuron for each input parameter in the model. The second layer is the pattern layer and contains a neuron for each training case. Both the summation and output layers consists of only one neuron. Execution starts by simultaneously presenting the input vector to all pattern layer neurons. Each pattern layer neuron computes a distance measure between the input and the training case represented by that neuron. It then subjects that distance measure to the neuron's activation function, which is essentially the Parzen window associated with the network's kernel. The neuron in the summation layer sums the pattern layer neurons. The attained activation of this neuron is the estimated density function value. The output layer delivers the prediction at the PNN level.

PNNs offer many advantages. While some deviation from normality is tolerated, large deviations usually cause problems for most standard multivariate statistical predictors (including predictors associated with multivariate linear and non-linear regression models). In particular, multi-modal distributions cause even most non-parametric methods to fail. Multiple-layer feed-forward networks, including the PNNs, can typically handle even the most complex distributions. Another reason to prefer PNN is if the data are likely to contain outliers, points that are very different from the majority. Outliers are generally more of a threat to other neural network models, and they can totally devastate many traditional statistical techniques. For the PNN the outliers have no real effect on decisions regarding to the more frequent cases, yet they will be properly handled if they are valid data. Usually, for most multiple-layer feed-forward networks (backpropagation networks for example) little is known about how they operate and what behavior is theoretically expected of them: they act as black boxes. The PNN, on the other hand, has superb mathematical credentials, is several order of magnitude faster than most multiple-layer feed-forward networks, and performs at least as well or better than they can do.

## The PNN-based prediction methodology for the toxicity of chemicals to the fathead minnow *Pimephales promelas*

The input required for prediction by our methodology consists of the logarithm of molecular weight, the values associated with the molecular descriptors in Table 1, the number of C, H, As, Br, Cl, F, Fe, Hg, I, K, Mn, N, Na, O, P, S, Se, Si, Sn, and Zn atoms present in the molecule, and the logarithm of the ratio of the molecular weight corresponding to all atoms present over the total molecular weight. The output consists of predicted 96-hours LC50 acute toxicity values for the fathead minnow in pT notation. Our actual version of the PNN-based prediction system for the acute toxicity of chemicals to the fathead minnow is founded on the 865 compounds data set resulted from querying the TerraTox™ toxicity database (TerraBase, 1998) for the availability of 96-hr LC50 acute toxicity of chemicals to the fathead minnow expressed in pT units. The list of these compounds with both measured and predicted 96-hours LC50 pT values is presented in Appendix 1.

For reasons discussed in Niculescu, Kaiser and Schüürmann (1998), we use the basic PNN with Gaussian kernel and data pre-processing consisting of a combination of Z-transform, hyperbolic transform and convenient linear compression functions. Creating the prediction system involved the following two preliminary research steps:

- (a) The analysis of the residuals (differences between the real, measured toxicity endpoints and the corresponding values predicted by the PNN) when the network is trained on all data indicate good predictive capabilities.
- (b) To prove that the good behavior of the preliminary PNN modeling experiment is not by chance, and that in fact the PNN is the right instrument to be used in computing acute toxicity values to the fathead minnow a cross-validation experiment was performed. For that purpose, the whole data set the 865 compounds was randomly split into five disjoint subsets, each containing 20% of the data. For each of these subsets, a PNN was trained based on the complementary 80% of the data. Then the fitted models were used to predict values for compounds *not used in the training* (i.e. the 20%). Finally, the predictions resulted from repeating the procedure for all five subsets were put together (resulting in a predicted value for each of the 865 compounds from a training set it was not part of) and then compared with the expected, in fact, measured data. The associated statistical indicators, presented in Kaiser and Niculescu (1998), suggest the fact that not only the PNN is appropriate to handle the prediction operation of the toxicity to the fathead minnow, but it is also stable and accurate.

As we can observe from Figure 2, presenting the flow chart of the methodology, the prediction process involves five stages. The first stage consists in pre-processing the input data in order to satisfy the input requirements associated with the Probabilistic Neural Network simulator computer program: an improved version of the one presented by

Masters (1995). The second stage handles the prediction at the PNN level. The five PNNs included in this part of the methodology are in fact the five cross-validation PNNs trained during the preliminary research. The pre-processed input is fed into each of the five PNNs which in turn generate a predicted value. The third stage consists in back-processing these five predictions in order to translate them into pT units. The actual toxicity value returned by the methodology is computed in the fourth stage from the five partial predictions using a special smoothing technique fully described in Kaiser and Niculescu (1998). This smoothing procedure acts as a correction for the unequal representation of various classes of compounds in the training data for the five cross-validation PNNs. Figure 4 gives an idea about the excellent quality of the predictions. It is obvious from Figure 3, the very strong Gaussian character of the residuals produced by the methodology when performing predictions for the 865 compounds data set. This observation justifies the use of the *t*-distribution in computing approximate 95% confidence intervals for the toxicity predictions based on the linear regression model of the measured over predicted values corresponding to the compounds in the 865 data set.

### **Advantages of using the PNN-based prediction methodology for the estimation of the toxicity of chemicals to the fathead minnow**

The advantages of using the PNN methodology are as follows:

- (1) the PNN methodology implements truly a structure-activity system using only molecular descriptors and the number of occurrences of a carefully selected set of molecular fragments;
- (2) no more need to classify chemicals into various substance classes;
- (3) no more need to identify potential or actual type of use of chemical;
- (4) no more need for partitioning and/or solubility information (octanol/water or similar partition coefficients, solubility in water, etc.);
- (5) gives one answer only for each structure;
- (6) the methodology is practically valid for all compounds sharing the same structural characteristics as those included in the 865 compounds used for building the PNN.

### **Limitations of the methodology**

One of the characteristics of the Artificial Intelligence systems based on learning is their sensitivity to the family properties of the training data. That means that these systems will perform properly only when the input data share the general family specific characteristics with the data used for training. If the system is used to compute toxicity for a compound from a class of substances absent or very poorly represented inside the 865 data set and uses a completely different toxicity mechanism, then the prediction may

not be reliable. Such types of substances would include, for example, complex peptide fragments, for which no measured fish toxicity values are available.

## **Comparisons with other methodologies**

There are other methodologies which can make estimates of the toxicity of chemicals to fathead minnow based on the structure of the chemicals, for example, TOPKAT and ECOSAR. The former uses primarily multiple linear correlations, the latter uses the octanol/water partition coefficient and derives a toxicity estimate from a linear correlation between the partition coefficient and toxicity value. This approach works well only in narrow sets of compounds whose mode of toxic action does not vary from the one used to develop the model and for which there are no functional groups interacting with each other. "Similarity" of the chemical structure alone, does not guarantee in any way the results as it is well known for some simple series of compounds that the mechanism of action changes suddenly with increasing substitution as in, for example, the chloronitrophenol series, while the octanol/water partition coefficient increases smoothly in this series. Furthermore, even the prediction of the octanol/water partition coefficient - and there are a number of commercially available programs can be fraught with gross errors. For example, we have compared the octanol/water partition coefficients computed for a variety of substances with the ACDLOGP (vers. 3.60) and KOWWIN (vers. 1.60) programs and find surprisingly large differences of over 4 orders of magnitude between them for some compounds. In contrast to those programs, which assume linear relationships between input and output, the PNN methodology does not make any such inherent assumption and can use non-linear relationships in its learning process. Therefore, when trying to predict effects of many different chemicals in the large universe of structures, no prior knowledge of the mechanism of activity needs to be assumed and the octanol/water partitioning does not enter explicitly into the prediction process.

## **Ways to improve the methodology in the near future**

At the present time we foresee at least the following two potential ways to improve the predictive capabilities of the above described methodology:

- (1) improving the input information through additional molecular descriptors relevant to the toxicity mechanism;
- (2) improving the input information through descriptors for relative structure fragment information;
- (3) adding measured data to enlarge the training set, particularly with substances which are not well or not proportionally represented in order to create a better image of the chemical universe.

## References

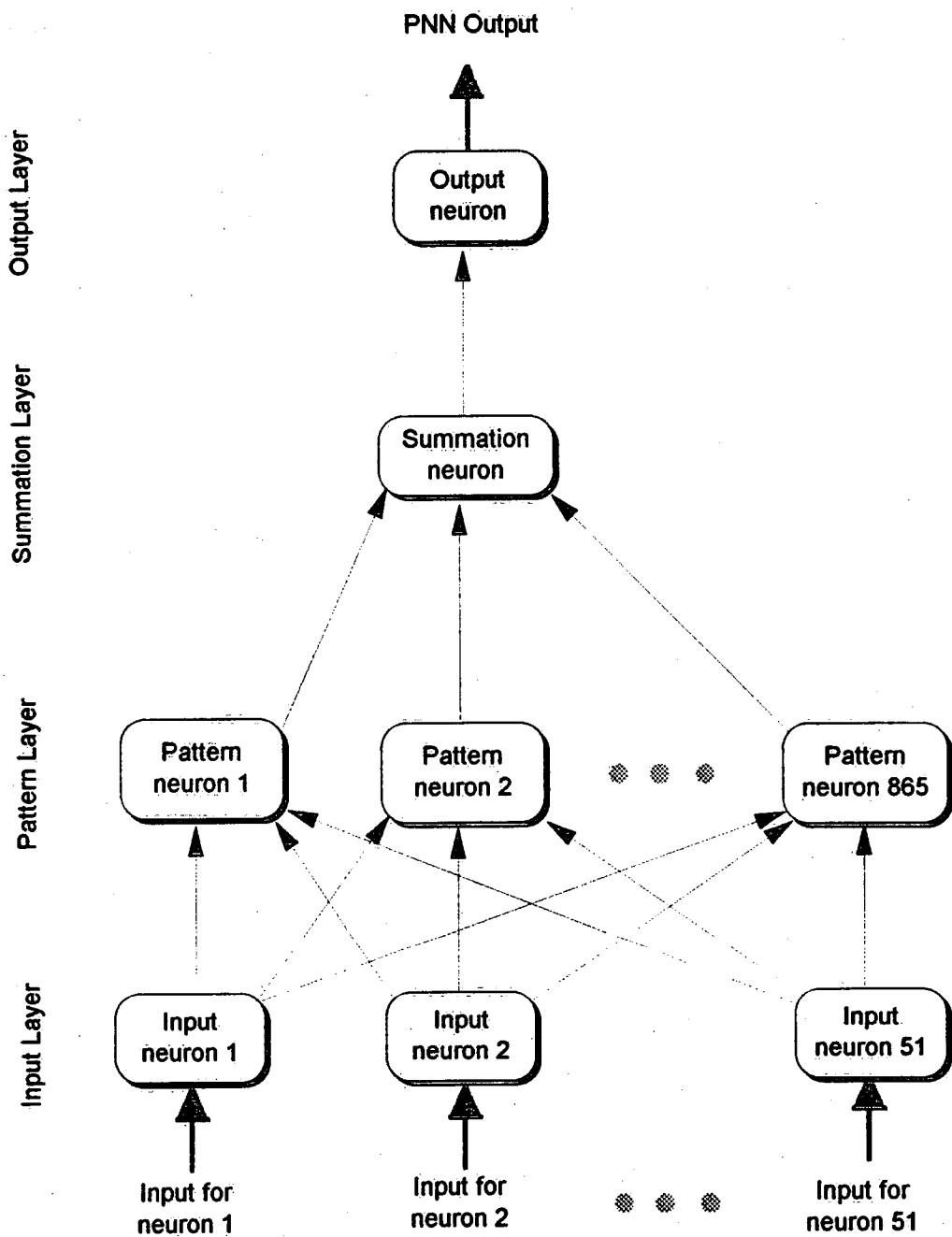
- Devillers, J., (ed.), (1996a). *Neural Networks in QSAR and Drug Design*. Academic Press, London.
- Devillers, J., (ed.), (1996b). *Genetic Algorithms in Molecular Modeling*. Academic Press, London.
- Kaiser, K.L.E.; Niculescu, S.P. (1998a). Using probabilistic neural networks to model the toxicity of chemicals to the fathead minnow (*Pimephales promelas*): A study based on 865 compounds. *Chemosphere*, in press.
- Kaiser, K.L.E.; Niculescu, S.P., (1998b). Neural network modeling of *Vibrio fischeri* toxicity data with structural physico-chemical parameters and molecular indicator variables. Poster, *Eighth International Workshop on QSAR in Environmental Sciences*, Baltimore, MD, May 16-20.
- Kaiser, K.L.E.; Niculescu, S.P.; Gough, K.M., (1998). Neural network modeling of *Vibrio fischeri* and fathead minnow acute toxicity data with molecular indicator variables and physico-chemical bulk parameters. Poster, *Workshop on Computational Methods in Toxicology*, Dayton, OH, April 20-22.
- Kaiser, K.L.E.; Niculescu, S.P.; McKinnon, M.B. (1997a). On the simple linear regression, multiple linear regression and the elementary probabilistic neural network with Gaussian kernel's performance in modeling toxicity values to fathead minnow based on Microtox data, the octanol/water partition coefficient and various structural descriptors for a 419 compounds data set. Pages 285-297 in: *Quantitative Structure-Activity Relationships in Environmental Sciences - VII*, Editors: F. Chen and G. Schüürmann, SETAC Press, Pensacola, FL.
- Kaiser, K.L.E.; Niculescu, S.P.; Schüürmann, G. (1997b). Feed forward backpropagation neural networks and their use in predicting the acute toxicity of chemicals to the fathead minnow. *Water Quality Research Journal of Canada* 32:637-657.
- Masters, T. (1993). *Practical Neural Network Recipes in C++*. Academic Press, San Diego.
- Masters, T. (1995). *Advanced Algorithms For Neural Networks. A C++ Sourcebook*. Wiley, New York.
- Meisel, W. (1972). *Computer-Oriented Approaches to Pattern Recognition*. Academic Press, New York.
- Nendza, M.; Russom, C.L. (1991). QSAR modelling of the ERL-D fathead minnow acute toxicity database. *Xenobiotica* 21:1065-1076.
- Niculescu, S.P.; Kaiser, K.L.E.; Schüürmann, G. (1998). Influence of data preprocessing and kernel selection on probabilistic neural network modeling of the acute toxicity of chemicals to the fathead minnow and *Vibrio fischeri* bacteria. *Water Quality Research Journal of Canada* 33:153-165 (1998).
- Specht, D.F. (1990). Probabilistic Neural Networks. *Neural Networks* 3:109-118.
- Specht, D.F.; Shapiro, P.D. (1991). Generalization accuracy of Probabilistic Neural Networks compared with back-propagation networks. *Lockheed Missile & Space Co. Inc. Independent Research Project RDD 360*, I-887-I-892.

TerraBase Inc. (1998). *The TerraTox™ & TerraFit™ Software Suite*. CD-ROM, v. 1.502  
TerraBase Inc., 3350 Fairview St., Suite 160, Burlington, Ontario L7N 3L5,  
Canada.

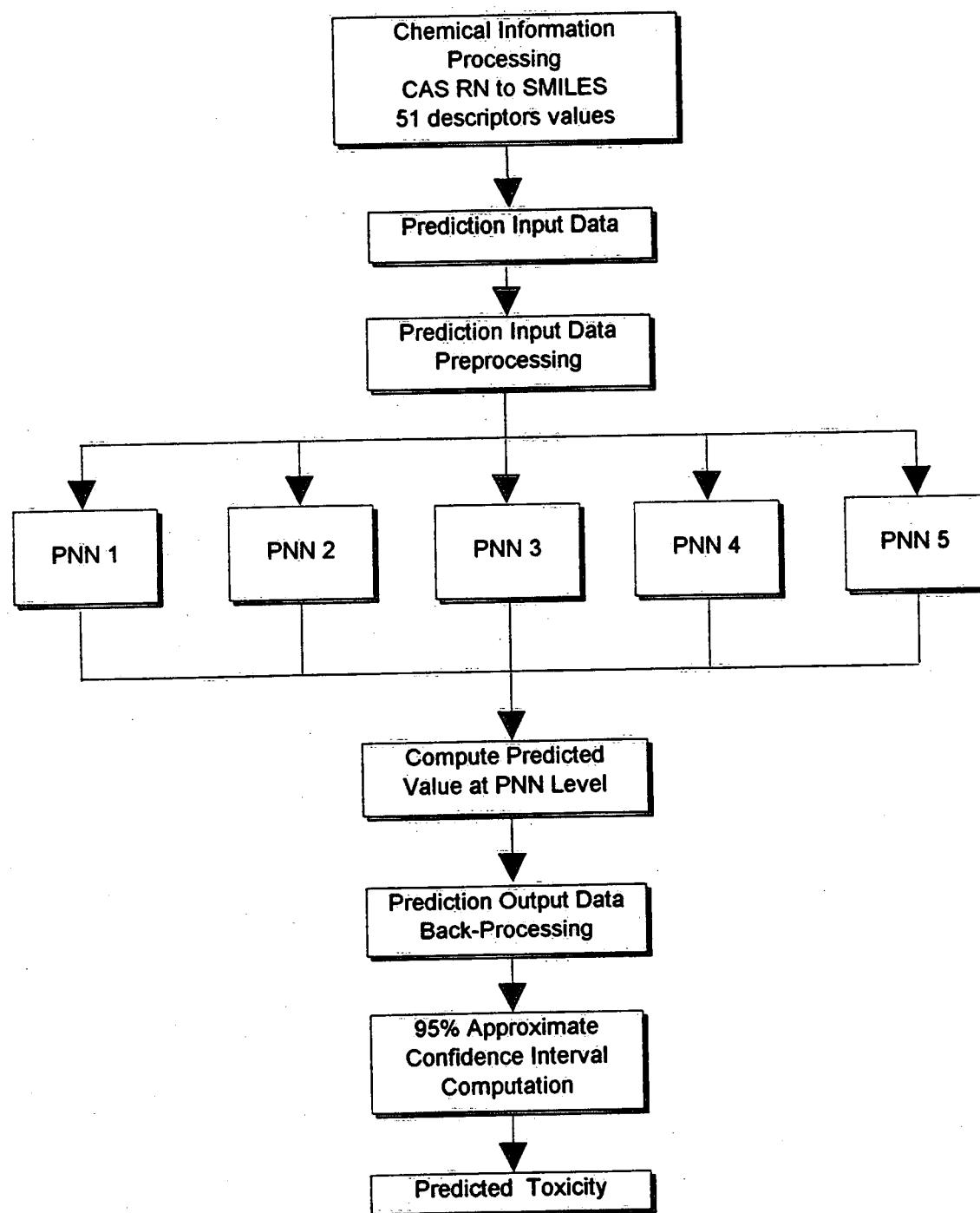
**Table 1. Functional group descriptors used by the methodology**

Group	Description
5ringY	aromatic (two double bonds) 5-rings containing one or more hetero atoms (e.g. N, O, S);
6ringY	aromatic (three double bonds) 6-rings containing one or more hetero atoms (e.g. N, O, S);
ar-OH	aryl hydroxy (-OH), sulphydryl (-SH), and -O-Na+ groups;
alk-OH	alkyl hydroxy (-OH) groups, includes -OH in =N-OH, S-OH, Se-OH, As-OH, Sn-OH, B-OH groups;
=O	keto ( $>C=O$ ) groups, includes =O in As=O, P=O, Se=O, S=O, and -N=O (nitroso) groups;
-COOH	acid groups where C= C, S, P, As, B, Se, Sn;
-COOR'	ester groups where C= C, S, P, As, B, Se, Sn;
-CONH2	amide groups where C= C, S, P, As, B, Se, Sn;
ar-NH2	aryl amino (-NH2) groups;
alk-NH2	alkyl amino (-NH2) groups;
-NO2	nitro (NO2) groups;
-CN	cyano (-CN) groups;
ar-X	halide atoms on aromatic rings or other $sp^2$ carbon atoms with X = Br, Cl, and/or I, but not F;
alk-X	alkyl halide (Alk-X) where X = Br, Cl, and/or I, but not F;
-CF3	trifluoromethyl (CF3) groups;
-F	number of aryl and/or alkyl fluoride (Ar-F and/or Alk-F) groups, other than in CF3 groups;
6ring	aromatic 6 member rings, excluding those containing nitrogen, sulfur and oxygen;
5ring	aromatic 5 member rings, excluding those containing nitrogen, sulfur and oxygen;
-O-	ether (R-O-R') linkages;
=CR2	number of terminal (=CR2) groups where R = H, Cl or Br;
other	structural moiety not expressed elsewhere on this list;
thio	sulfide bridge;
thion	sulfoxide bridge;
SOx	sulfoxide (-SO-), sulfon (-SO2-), sulfate (-OSO3-), selenoxide (-Se-O-), and/or selenone (-SeO2-) groups;
POx	phosphate [P(O)-(OR)x], phosphite [P(OR)x], arsenate [As(O)-(OR)x], and/or (B-OR)x groups;
-N=	$sp^2$ hybridized nitrogen atoms, such as in azo (-N=N-), (=N-N=), azoxy (-N=N(O)-), and includes (=N+=) in aromatic dye compounds;
metal(no C)	inorganic component without bond to carbon atom;
ionic	ionic state;
Organotin	compound is organo-metallic;
=CH-CO-	compound is conjugated to produce an acidic (CH) group; e.g. =CH-C(=O)-R;
i-but	tertiary butyl (value 1) or isopropyl (value 0.5) group;
n-C	the longest aliphatic chain, not terminating with an aromatic ring, carboxy group or other large substituent;
-yne	number of carbon-carbon triple bonds (acetylenic bonds) in the compound.

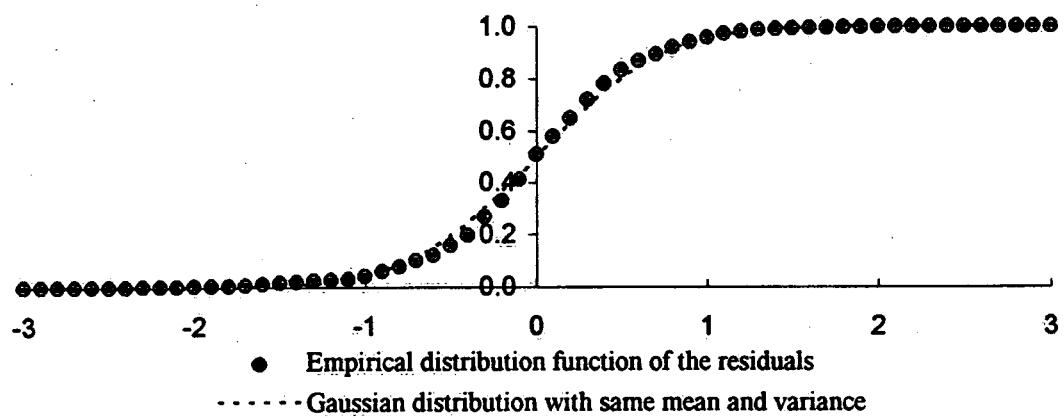
**Figure 1.** Architecture of the Probabilistic Neural Networks involved in the prediction methodology for 96-hr LC50 toxicity values of chemicals to the fathead minnow *Pimephales promelas*



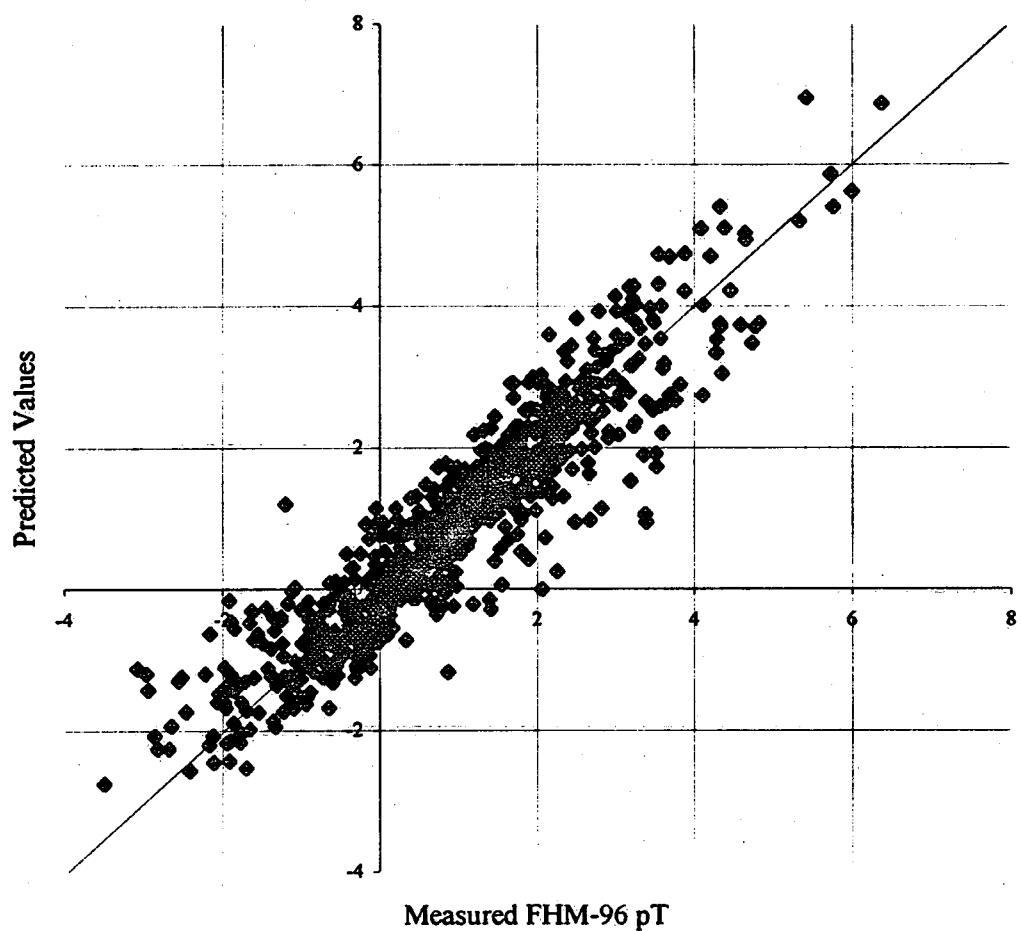
**Figure 2.** Flow chart diagram of the PNN-based methodology for the prediction of 96-hr LC50 toxicity values of chemicals to the fathead minnow *Pimephales promelas*



**Figure 3.** Comparison between the empirical distribution of the residuals generated by the methodology and the Gaussian distribution with the same mean and variance



**Figure 4.** Plot of the values predicted by the methodology versus measured values for the 865 compounds data set



**Appendix 1. List of substances used to build the predictive methodology for the toxicity to the fathead minnow and the associated measured and predicted values**

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
50-00-0	0.1	-0.662	67-63-0	-2.21	-1.200
50-06-6	-0.32	-0.431	67-64-1	-2.15	-0.636
50-29-3	4.46	4.217	67-66-3	0.23	0.238
51-28-5	1.29	1.303	67-68-5	-2.64	-1.939
51-79-6	-1.77	-2.168	67-72-1	2.2	1.290
52-68-6	1.51	1.976	68-12-2	-2.16	-2.204
54-21-7	-0.93	-1.634	70-30-4	4.29	3.528
55-18-5	-0.88	-1.452	70-69-9	0.01	0.247
55-21-0	-0.74	-0.830	71-23-8	-1.88	-1.206
55-38-9	2.06	3.027	71-36-3	-1.37	-0.847
56-23-5	0.55	0.511	71-41-0	-0.73	-0.518
56-35-9	5.34	5.202	71-43-2	0.62	0.732
56-37-1	0.15	0.193	71-55-6	0.45	0.339
56-38-2	2.35	2.751	71-73-8	1	0.970
57-06-7	3.06	2.612	72-20-8	5.77	5.405
57-14-7	0.88	-1.180	72-43-5	4.66	4.932
57-15-8	0.12	0.006	75-05-8	-1.61	-0.322
57-33-0	0.7	0.759	75-07-0	0.15	-0.558
57-43-2	0.42	-0.131	75-09-2	-0.56	0.115
57-74-9	3.55	4.730	75-21-8	-0.28	-0.891
58-08-2	0.11	-0.457	75-31-0	-1.59	-1.255
58-27-5	3.2	1.537	75-35-4	-0.05	0.920
58-89-9	3.52	1.921	75-36-5	0.27	-0.162
58-90-2	2.35	2.684	75-47-8	2.13	2.349
59-50-7	1.4	1.635	75-57-0	-0.62	-0.802
59-97-2	-0.25	-0.547	75-65-0	-1.94	-1.374
60-00-4	0.69	0.395	75-89-8	-0.08	-0.743
60-13-9	1.1	1.558	75-97-8	0.07	-0.253
60-29-7	-1.54	-0.636	76-01-7	1.44	1.029
60-41-3	2.54	2.918	76-03-9	-1.09	-1.691
60-57-1	4.33	5.405	76-22-2	0.24	0.098
62-53-3	0	0.013	76-44-8	4.21	4.702
62-55-5	-0.56	-0.829	76-87-9	4.83	3.757
62-73-7	1.74	1.905	77-47-4	4.59	3.735
62-75-9	-1.1	-1.631	77-71-4	-2.11	-2.074
63-25-2	1.36	1.607	77-73-6	1.04	0.822
64-17-5	-2.51	-1.246	77-74-7	-0.82	-0.773
64-19-7	-0.12	-0.942	77-75-8	-1.1	-0.034
65-30-5	1.24	1.226	78-27-3	-0.31	0.142
65-45-2	0.13	-0.248	78-51-3	1.55	1.896
65-85-0	0.01	-0.313	78-59-1	-0.22	-0.244
66-25-1	0.75	0.186	78-83-1	-1.3	-1.369
66-76-2	1.82	2.255	78-87-5	-0.05	0.240
67-36-7	1.63	1.617	78-90-0	-1.13	-1.237
67-56-1	-2.95	-1.205	78-92-2	-1.41	-1.128

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
78-93-3	-1.65	-0.479	90-59-5	2.52	2.543
78-96-6	-0.64	-1.686	91-20-3	1.32	1.190
78-97-7	1.9	0.421	91-22-5	0.22	0.448
79-00-5	0.21	0.339	91-23-6	-0.04	1.140
79-01-6	0.47	1.318	91-65-6	0.86	0.792
79-06-1	-0.19	-0.827	91-66-7	0.96	0.578
79-19-6	0.64	0.011	91-88-3	0.53	0.234
79-20-9	-0.64	-0.295	92-52-4	1.9	1.430
79-34-5	0.92	0.673	92-88-6	1.05	1.476
79-95-8	2.44	3.444	93-89-0	1.14	1.006
80-05-7	1.7	1.805	93-91-4	2.21	1.457
80-46-6	1.8	2.015	94-09-7	0.66	0.759
80-52-4	0.42	0.151	94-62-2	1.56	1.782
80-62-6	-0.41	0.502	94-67-7	1.63	1.570
81-19-6	2.37	2.938	94-68-8	0.5	0.379
83-32-9	1.95	1.658	94-75-7	-0.08	0.117
83-34-1	1.17	0.856	94-81-5	1.32	1.241
83-79-4	3.44	3.973	95-01-2	1.02	1.134
84-62-8	3.6	2.212	95-16-9	0.33	0.353
84-66-2	0.84	1.779	95-47-6	0.81	0.908
84-74-2	2.4	2.637	95-48-7	0.77	0.915
85-00-7	1.39	1.341	95-49-8	1.23	1.443
85-47-2	-0.38	-0.547	95-50-1	1.4	1.968
85-68-7	2.13	2.711	95-51-2	1.34	1.010
86-50-0	3.69	4.693	95-52-3	0.75	0.937
86-57-7	1.28	1.277	95-53-4	0.63	0.077
87-17-2	1.73	1.201	95-57-8	1.02	1.597
87-61-6	1.89	2.299	95-63-6	1.21	1.033
87-68-3	3.42	2.616	95-65-8	0.94	0.991
87-72-9	-2.4	-2.568	95-73-8	1.54	2.030
87-86-5	3.06	2.765	95-75-0	1.74	2.030
87-91-2	-0.5	-0.034	95-76-1	1.36	1.755
88-06-2	1.85	2.533	95-80-7	-1.07	0.022
88-30-2	1.36	1.451	95-82-9	2.1	1.755
88-68-6	-0.46	-0.808	95-94-3	2.85	2.519
88-72-2	0.57	0.972	95-95-4	1.86	2.533
88-73-3	0.73	1.205	96-05-9	2.11	0.737
88-75-5	0	0.775	96-13-9	0.49	0.484
88-85-7	2.54	2.423	96-17-3	0.94	-0.242
89-61-2	1.1	1.623	96-18-4	0.35	0.483
89-62-3	0.79	0.835	96-22-0	-1.25	-0.392
89-83-8	1.67	1.743	96-29-7	-0.99	-1.271
90-02-8	1.73	1.127	96-80-0	-0.14	-0.612
90-12-0	1.2	1.295	97-02-9	1.07	1.279
90-15-3	1.53	1.224	97-23-4	2.94	3.347
90-43-7	1.45	1.427	98-01-1	0.67	-0.221
90-47-1	1.73	1.698	98-04-4	0.04	-0.237

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
98-08-8	1.09	1.250	104-76-7	0.66	0.474
98-54-4	1.47	1.758	104-88-1	1.81	1.661
98-56-6	1.76	1.970	104-90-5	0.17	-0.557
98-82-8	1.28	1.124	105-14-6	-0.33	0.308
98-86-2	-0.13	0.715	105-53-3	1.03	0.752
98-88-4	0.62	0.937	105-60-2	-1.75	-1.598
98-95-3	0.01	0.898	105-67-9	0.86	0.991
99-03-6	-0.45	0.095	105-75-9	2.6	2.506
99-08-1	0.63	0.972	105-99-7	1.85	2.207
99-35-4	2.29	1.909	106-40-1	0.56	0.609
99-52-5	0.24	0.835	106-42-3	1.21	0.908
99-55-8	0.35	0.835	106-43-4	1.33	1.443
99-61-6	1.41	1.315	106-44-5	0.58	0.915
99-65-0	1.38	1.702	106-46-7	1.62	1.968
99-88-7	1.13	0.617	106-47-8	0.62	1.010
99-97-8	0.44	0.313	106-48-9	1.32	1.597
99-99-0	0.76	0.972	106-49-0	-0.14	0.077
100-01-6	0.04	0.769	106-51-4	3.38	1.060
100-02-7	0.57	0.775	106-63-8	1.79	1.811
100-10-7	0.51	0.251	106-89-8	0.86	0.073
100-25-4	2.22	1.702	106-94-5	0.26	0.592
100-37-8	-1.18	-1.509	107-02-8	3.53	1.735
100-41-4	0.4	0.916	107-05-1	0.5	1.105
100-42-5	1.41	1.193	107-06-2	-0.14	0.152
100-44-7	1.4	1.129	107-07-3	0.34	-0.728
100-46-9	0.02	-0.138	107-10-8	-0.72	-0.967
100-47-0	0.21	0.177	107-12-0	-1.44	-0.273
100-51-6	-0.63	-0.212	107-13-1	0.47	-0.132
100-52-7	1.14	0.698	107-14-2	1.75	0.781
100-61-8	0.03	0.077	107-15-3	-0.28	-1.140
100-64-1	-0.26	-1.109	107-18-6	2.26	0.251
100-70-9	-0.84	-0.930	107-19-7	1.56	0.054
100-71-0	-0.59	-0.687	107-21-1	-2.93	-1.430
100-79-8	-2.1	-2.450	107-22-2	-0.57	-0.587
100-97-0	-2.55	-1.305	107-29-9	-0.11	-1.123
101-84-8	1.63	1.482	107-41-5	-1.96	-1.109
102-08-9	1.08	1.037	107-45-9	0.72	-0.197
102-27-2	0.44	0.379	107-47-1	0.7	1.412
102-69-2	0.45	0.958	107-49-3	2.18	2.104
102-71-6	-1.9	-2.150	107-87-9	-1.16	-0.204
103-05-9	0.39	0.840	108-05-4	0.57	0.421
103-76-4	-1.69	-1.716	108-10-1	-0.71	-0.209
103-83-3	0.55	0.169	108-20-3	-0.89	-0.428
103-90-2	-0.73	-0.360	108-38-3	0.82	0.908
104-13-2	1.17	0.952	108-39-4	0.29	0.915
104-40-5	3.2	3.161	108-41-8	0.84	1.443
104-51-8	1.83	1.441	108-46-3	0.04	0.950

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
108-59-8	1.03	0.495	111-42-2	-1.65	-1.987
108-70-3	1.74	2.299	111-46-6	-2.85	-2.079
108-86-1	0.89	1.333	111-47-7	0.74	1.240
108-88-3	0.43	0.803	111-68-2	0.72	0.564
108-89-4	-0.64	-0.772	111-69-3	-1.25	-0.447
108-90-7	0.7	1.403	111-70-6	0.53	0.240
108-93-0	-0.85	-1.042	111-76-2	-0.96	-1.033
108-94-1	-0.81	-0.489	111-83-1	2.36	2.178
108-95-2	0.51	0.883	111-86-4	1.4	1.034
108-99-6	-0.19	-0.772	111-87-5	1	0.657
109-01-3	-1.36	-1.242	111-90-0	-1.94	-2.173
109-06-8	-0.98	-0.772	111-91-1	-0.03	0.122
109-07-9	-1.35	-1.242	111-96-6	-1.81	-1.389
109-21-7	1.1	0.981	112-05-0	0.18	-0.176
109-60-4	0.23	0.154	112-12-9	2.06	1.597
109-64-8	2.05	1.391	112-18-5	3.39	2.651
109-65-9	0.57	0.931	112-20-9	1.82	1.473
109-73-9	-0.56	-0.685	112-24-3	-3.07	-1.131
109-75-1	-0.43	-0.239	112-27-6	-2.67	-2.255
109-76-2	-1.21	-1.237	112-30-1	1.84	1.408
109-77-3	2.07	-0.006	112-34-5	-0.9	-0.179
109-85-3	-0.84	-1.172	112-42-5	2.22	1.687
109-86-4	-2.45	-1.741	112-53-8	2.27	1.896
109-87-5	-1.96	-1.603	112-80-1	0.14	0.741
109-89-7	-1.07	-1.016	114-26-1	1.37	1.747
109-97-7	-0.5	-0.938	115-19-5	-1.59	-0.714
109-99-9	-1.48	-0.768	115-20-8	-0.3	-0.220
110-00-9	0.05	-0.421	115-29-7	5.43	6.952
110-06-5	2.11	1.539	115-32-2	2.79	3.923
110-12-3	-0.14	-0.198	115-86-6	2.57	1.981
110-40-7	1.98	2.285	116-06-3	3.83	2.898
110-43-0	-0.06	0.351	117-80-6	3.18	2.787
110-54-3	1.54	0.581	118-55-8	2.26	1.823
110-56-5	0.39	0.343	118-61-6	0.93	0.991
110-58-7	-0.31	-0.318	118-74-1	4.11	2.734
110-62-3	0.84	-0.062	118-79-6	1.7	2.706
110-65-6	0.21	-0.088	118-96-7	1.88	1.902
110-73-6	-1.22	-1.738	119-32-4	0.77	0.835
110-80-5	-1.95	-1.682	119-34-6	0.65	0.892
110-86-1	-0.1	-0.800	119-61-9	1.08	1.557
110-88-3	-1.82	-2.106	120-07-0	-0.61	-0.139
110-93-0	0.17	-0.134	120-21-8	0.87	0.619
111-13-7	0.54	0.664	120-62-7	2.64	3.103
111-15-9	0.5	0.442	120-80-9	1.08	0.950
111-25-1	1.68	1.680	120-82-1	1.78	2.299
111-26-2	0.25	0.104	120-83-2	1.32	2.239
111-27-3	0.02	-0.157	120-92-3	-1.33	-0.592

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
121-14-2	0.75	1.723	140-88-5	1.6	1.307
121-32-4	0.29	0.918	141-03-7	1.71	2.071
121-33-5	0.23	0.985	141-28-6	1.05	1.450
121-54-0	2.45	2.591	141-43-5	-1.53	-1.750
121-57-3	0.24	-0.074	141-78-6	-0.42	-0.175
121-69-7	0.19	0.176	141-91-3	-0.53	-0.982
121-73-3	0.92	1.205	141-93-5	1.51	1.213
121-82-4	1.24	1.497	141-97-9	-0.36	0.294
121-87-9	0.96	1.027	142-28-9	-0.06	0.240
122-03-2	1.35	1.039	142-62-1	-0.44	-0.858
122-14-5	1.94	2.544	142-71-2	2.67	2.649
122-39-4	1.65	0.704	142-92-7	1.52	1.067
122-99-6	-0.4	-0.422	142-96-1	0.6	0.794
123-07-9	1.07	1.005	143-08-8	1.4	1.059
123-15-9	0.73	0.153	143-16-8	2.38	2.307
123-31-9	3.4	0.950	143-33-9	2.46	2.269
123-42-2	-1.84	-0.567	143-50-0	3.16	3.528
123-54-6	0.02	-0.573	148-18-5	1.41	1.649
123-66-0	1.21	1.067	148-53-8	1.8	0.985
123-72-8	0.65	-0.160	150-19-6	0.21	0.783
123-86-4	0.81	0.502	150-76-5	0.05	0.783
123-91-1	-2.05	-1.601	150-78-7	0.07	0.540
124-04-9	-1.85	-1.894	151-21-3	1.64	1.690
124-22-1	3.26	2.362	152-16-9	0.46	0.326
125-12-2	1.58	1.625	253-52-1	0.11	0.170
126-73-8	1.51	1.897	260-94-6	1.89	1.540
126-81-8	-1.91	-0.160	271-89-6	0.93	0.912
127-00-4	-0.41	-0.719	280-57-9	-1.19	-1.291
127-06-0	-0.88	-1.135	281-23-2	2.68	0.981
127-18-4	1.09	1.699	298-00-0	1.47	2.442
127-20-8	-0.25	-0.575	298-02-2	3.02	3.586
127-65-1	1.49	1.288	298-03-3	1.95	2.995
127-66-2	0.11	0.362	298-04-4	2.16	3.598
128-37-0	2.78	2.902	299-84-3	3.02	3.921
128-44-9	-1.91	-2.428	300-76-5	2.06	2.481
129-67-9	-0.14	-0.760	309-00-2	4.65	5.030
131-11-3	0.21	1.139	309-43-3	1.04	0.980
131-52-2	3.14	3.919	311-45-5	3.04	3.429
132-64-9	1.97	1.939	314-40-9	0.15	-0.218
133-06-2	3.18	4.259	315-18-4	1.12	1.491
133-07-3	3	4.130	329-71-5	1.74	1.303
133-11-9	1.68	1.930	330-54-1	1.22	1.085
134-62-3	0.24	0.321	330-93-8	2.24	2.400
135-19-3	1.62	1.224	333-41-5	1.92	2.552
137-30-4	4.09	5.088	350-46-9	0.7	0.831
137-40-6	-1.69	-2.530	368-77-4	0.56	0.483
140-31-8	-1.23	-0.770	371-40-4	0.82	0.506

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
383-63-1	-1.85	-1.451	584-79-2	4.12	4.014
385-00-2	0.36	0.240	584-84-9	0.02	0.053
387-45-1	1.23	1.729	589-09-3	0.57	0.355
393-39-5	0.77	0.690	589-16-2	0.22	0.219
446-52-6	1.96	1.779	590-86-3	1.42	-0.288
447-60-9	0.61	0.483	591-78-6	-0.63	0.081
454-89-7	2.27	2.086	592-35-8	-0.92	-1.536
459-59-6	0.51	0.476	592-46-1	0.61	0.073
464-45-9	0.38	0.104	592-85-8	3.32	3.674
464-48-2	0.95	0.486	593-08-8	2.74	2.011
470-82-6	0.18	0.261	596-85-0	3.38	3.464
471-77-2	2.25	2.546	597-64-8	4.33	3.753
475-20-7	1.3	1.205	598-74-3	-0.51	-1.005
496-16-2	0.17	0.766	600-36-2	-0.15	-0.646
497-37-0	-0.31	-0.938	602-01-7	2.01	1.723
498-66-8	0.97	0.240	603-83-8	0.48	0.835
499-83-2	-0.29	-1.078	606-20-2	0.99	1.723
500-22-1	0.81	-0.244	607-00-1	0.82	0.479
502-56-7	0.66	0.875	607-81-8	1.66	2.153
506-96-7	0.48	0.089	608-71-9	3.72	2.751
512-56-1	-1.7	-1.309	608-93-5	3	2.654
513-81-5	1.08	0.720	609-23-4	2.59	2.965
514-10-3	2.1	2.546	610-39-9	2.08	1.723
525-82-6	1.8	1.778	613-45-6	0.92	0.950
527-60-6	1.02	1.098	614-80-2	0.73	-0.360
528-29-0	2.45	1.702	615-65-6	0.6	0.974
529-19-1	0.42	0.275	616-21-7	0.62	0.343
529-20-4	0.36	0.782	616-45-5	-2.81	-2.257
532-32-1	-0.53	-1.223	616-86-4	0.85	1.122
534-52-1	2.05	1.377	618-85-9	0.91	1.723
538-68-1	1.94	1.692	618-87-1	0.93	1.279
540-88-5	-0.45	-0.325	619-15-8	2.15	1.723
541-73-1	1.3	1.968	619-50-1	0.89	1.243
542-75-6	2.67	1.637	619-72-7	0.78	1.090
544-40-1	1.61	1.532	619-80-7	0.1	0.103
552-41-0	0.38	0.918	620-88-2	1.91	1.708
552-89-6	1.02	1.315	621-08-9	0.46	0.284
555-16-8	1.18	1.315	621-42-1	-0.87	-0.360
563-12-2	2.73	3.542	622-40-2	-1.32	-1.948
563-47-3	1.99	1.117	623-25-6	2.65	1.790
563-80-4	-1	-0.288	625-86-5	0.13	-0.288
569-64-2	3.48	3.816	627-30-5	-0.93	-0.719
570-24-1	0.8	0.835	628-76-2	0.75	0.481
573-56-8	0.67	1.303	629-04-9	2.09	1.971
576-26-1	0.74	0.991	629-11-8	-1.85	-1.273
578-46-1	0.8	0.835	629-19-6	1.76	1.364
583-53-9	1.77	1.929	629-40-3	-0.59	-0.776

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
634-66-2	2.43	2.519	945-51-7	0.37	0.307
634-67-3	1.74	2.070	955-83-9	3.64	2.624
635-93-8	2.31	1.990	999-61-1	1.6	0.888
645-56-7	1.09	1.232	1071-83-6	0.25	-0.149
653-37-2	2.25	2.311	1072-97-5	-0.01	-0.423
683-72-7	-0.27	-0.770	1080-32-6	-0.17	0.926
685-91-6	-1.11	-1.312	1111-78-0	0.32	0.018
693-16-3	1.4	0.970	1122-54-9	-0.14	-0.255
693-54-9	1.44	1.307	1126-46-1	1.2	1.405
693-65-2	1.7	1.391	1126-79-0	1.42	1.380
693-93-6	-1.22	-0.951	1129-35-7	0.54	0.525
693-98-1	-0.54	-1.096	1194-65-6	1.46	1.645
700-38-9	0.51	0.861	1198-55-6	2.29	2.776
700-58-3	0.39	0.336	1204-21-3	3.69	2.738
706-14-9	0.98	0.945	1303-33-9	0.26	0.194
708-76-9	1.83	1.067	1330-20-7	0.87	0.908
709-98-8	1.4	1.412	1420-04-8	3.55	4.306
732-26-3	3.63	3.191	1444-64-0	0.6	0.747
760-23-6	1.25	1.145	1461-25-2	3.89	4.732
761-65-9	0.25	0.086	1482-15-1	-0.29	-0.609
764-01-2	0.84	0.005	1484-13-5	4.78	3.707
764-13-6	1.47	0.397	1484-26-0	1.34	1.116
768-94-5	0.78	-0.009	1563-66-2	2.42	1.954
769-28-8	-0.03	-0.641	1582-09-8	3.5	3.773
771-60-8	0.69	0.596	1600-27-7	3.22	4.101
786-19-6	3.16	3.880	1634-04-4	-0.88	-0.567
791-28-6	0.72	0.900	1638-22-8	1.47	1.610
815-57-6	-1.88	-0.459	1647-16-1	2.68	2.354
818-61-1	1.38	1.223	1689-82-3	2.26	2.449
818-72-4	2.49	0.952	1689-83-4	1.74	2.188
821-55-6	0.97	0.974	1689-84-5	1.35	1.800
822-86-6	0.92	0.664	1740-19-8	2.16	2.693
831-82-3	1.58	1.472	1745-81-9	0.95	1.078
868-77-9	-0.24	0.507	1746-23-2	2.51	2.372
868-85-9	-0.31	-1.255	1761-61-1	2.19	2.302
872-31-1	1.42	1.450	1787-61-7	1.88	1.541
874-42-0	1.99	2.193	1825-21-4	2.64	2.756
882-33-7	3.3	3.261	1871-57-4	2.82	1.145
886-86-2	0.52	0.424	1891-95-8	0.89	1.533
887-79-6	1.81	2.099	1912-24-9	1.16	1.028
920-66-1	-0.16	-0.667	1918-02-1	0.64	0.349
924-41-4	0.41	0.107	1929-82-4	1.35	1.989
927-74-2	0.29	0.005	1962-75-0	2.67	2.637
928-96-1	-0.58	-0.650	1965-09-9	1.54	1.525
928-97-2	-0.43	-0.650	2008-58-4	-0.39	-0.096
932-16-1	-0.11	-0.448	2016-57-1	2.18	1.844
939-23-1	0.98	0.914	2032-59-9	1.39	1.484

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
2034-22-2	1.81	2.004	4460-86-0	0.6	0.920
2104-64-5	3.61	3.126	4655-34-9	0.53	0.813
2117-11-5	0.38	0.228	4798-44-1	0.52	0.013
2138-22-9	1.96	1.800	4839-46-7	-1.95	-1.456
2150-47-2	0.57	0.992	4901-51-3	2.72	2.684
2176-62-7	2.73	2.403	4916-57-8	0.07	-0.158
2216-51-5	0.92	0.163	4920-77-8	0.52	0.861
2232-08-8	0.73	0.658	5217-47-0	-1.35	-1.865
2234-16-4	1.21	2.179	5267-27-6	1.92	1.321
2243-27-8	1.42	1.717	5292-45-5	1.56	1.477
2243-62-1	0.24	0.378	5329-14-6	0.14	-0.372
2357-47-3	0.78	0.688	5331-91-9	1.8	2.102
2362-61-0	0.6	0.747	5372-81-6	1.37	1.343
2370-63-0	0.76	0.926	5395-75-5	0.4	1.286
2416-94-6	1.22	1.098	5407-04-5	0.07	-0.432
2437-25-4	2.63	2.472	5465-65-6	1.56	1.786
2437-29-8	3.89	4.203	5600-21-5	0.02	-0.225
2439-77-2	0.1	-0.071	5673-07-4	0.88	0.712
2447-79-2	0.3	-0.096	5683-33-0	-0.02	-0.764
2455-24-5	0.69	1.030	5813-64-9	-0.74	-0.627
2460-49-3	1.64	2.173	5835-26-7	2.54	2.829
2463-84-5	2	2.531	5922-60-1	0.73	0.912
2495-37-6	1.58	1.583	5989-27-5	2.28	2.040
2499-95-8	2.16	2.178	6175-49-1	2.19	1.832
2626-83-7	1.32	1.619	6203-18-5	1.42	1.078
2759-28-6	0.57	0.248	6266-23-5	0.03	-0.399
2859-67-8	-0.04	-0.631	6284-83-9	3.09	2.899
2869-34-3	3.48	2.528	6358-64-1	1.54	1.682
2894-51-1	2.04	1.909	6361-21-3	1.72	1.732
2905-69-3	1.17	1.609	6393-42-6	1.18	1.321
2921-88-2	3.24	4.278	6575-09-3	1	1.194
2973-76-4	0.59	1.479	6602-32-0	-0.43	-0.906
3066-71-5	2.02	1.965	6636-78-8	-0.68	-1.079
3126-90-7	2.49	2.637	6921-29-5	-0.35	-0.307
3206-31-3	1.24	1.459	6948-86-3	-0.38	-0.423
3389-71-7	3.2	3.980	7173-51-5	2.89	3.228
3428-24-8	2.3	2.443	7209-38-3	-1.19	1.211
3481-20-7	2.92	2.230	7212-44-4	2.19	2.637
3558-69-8	3.04	2.185	7220-79-3	0.85	1.123
3689-24-5	3.26	4.013	7250-67-1	0.04	-0.375
3698-83-7	3.77	2.665	7307-55-3	2.91	2.138
3923-52-2	1.27	1.053	7383-19-9	1.8	0.536
3944-76-1	0.85	0.351	7447-40-7	-1.07	-1.361
4117-14-0	2.16	1.632	7447-41-8	0	-0.491
4214-79-3	-0.94	-1.079	7487-88-9	-1.37	-1.233
4253-89-8	1.26	1.381	7487-94-7	3.26	3.773
4412-91-3	-0.71	-1.251	7632-00-0	1.48	1.629

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted	CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
7646-85-7	1.35	1.396	16879-02-0	-0.22	-1.079
7647-14-5	-2.04	-1.478	16919-19-0	0.79	0.319
7664-41-7	0.98	0.038	17584-12-2	-0.89	-0.867
7718-54-9	1.4	-0.152	17754-90-4	1.56	1.240
7757-82-6	-1.75	-2.037	17804-35-2	2.12	2.424
7761-88-8	4.28	3.336	18278-34-7	1.02	0.985
7775-09-9	1.37	1.523	18292-97-2	3.37	1.902
7778-50-9	0.9	1.221	18368-63-3	-0.26	-0.396
7778-80-5	-0.59	-1.326	19406-51-0	1.46	1.321
7784-46-5	0.96	0.730	19549-98-5	0.46	0.022
7786-30-3	-1.35	-0.401	20662-84-4	-0.61	-0.781
7789-43-7	0.38	0.355	21725-46-2	1.17	1.215
8001-35-2	4.36	3.053	22037-97-4	1.38	1.586
10031-82-0	0.73	1.006	22104-62-7	1.19	-0.215
10043-52-4	-1.62	-0.310	22726-00-7	0.33	-0.033
10102-18-8	1.24	1.730	23103-98-2	0.08	0.002
10108-64-2	2.08	1.800	23135-22-0	1.42	2.274
10113-37-8	0.56	0.776	24019-05-4	1.92	1.885
10202-92-3	1.26	1.321	24544-04-5	1.03	1.319
10222-01-2	2.13	2.078	25154-52-3	3.21	3.161
10293-06-8	0.53	0.655	26628-22-8	1.08	1.226
10453-86-8	4.74	3.475	28001-58-3	0	-0.119
10543-57-4	-3.48	-2.753	28434-00-6	3.58	3.542
11067-81-5	1.21	1.559	28680-45-7	3.59	3.995
12125-01-8	-0.99	-1.130	29091-05-2	2.35	3.356
13071-79-9	4.34	3.717	29553-26-2	-0.56	-1.023
13171-21-6	0.48	0.313	30030-25-2	2.69	2.206
13209-15-9	2.98	3.016	31502-57-5	0.77	0.797
13356-08-6	5.74	5.864	34274-04-9	0.3	0.095
13410-01-0	1.69	1.752	34723-82-5	-0.06	0.472
13608-87-2	2.05	2.307	35367-38-5	2.86	3.317
13909-73-4	0.06	0.922	35572-78-2	1.12	1.321
13952-84-6	-0.58	-1.161	37529-30-9	3.57	2.583
14064-10-9	2.31	1.839	39145-47-6	2.11	2.205
14321-27-8	0.37	0.232	39905-57-2	1.78	1.965
14338-32-0	0.12	0.089	42087-80-9	0.89	1.264
14484-64-1	2.51	3.820	42454-06-8	0.6	0.907
14548-45-9	1.11	1.301	51630-58-1	6	5.618
14548-46-0	0.25	0.693	52645-53-1	4.39	5.101
14901-07-6	1.58	1.435	54576-32-8	1.47	1.586
14938-35-3	2.18	2.036	55792-61-5	2.77	3.141
15045-43-9	-0.12	0.146	56108-12-4	0.75	0.528
15128-82-2	-0.08	-0.119	56207-39-7	2.34	1.321
15673-00-4	-0.77	-0.776	56348-39-1	1.84	1.752
15972-60-8	1.73	1.931	56348-40-4	1.25	1.441
16245-79-7	3.24	2.305	57055-39-7	2.74	3.373
16752-77-5	1.89	2.517	59756-60-4	1.18	1.290

CAS Number	FHM-96 pT Measured	FHM-96 pT Predicted
61096-84-2	1.95	1.726
65337-13-5	0.78	0.005
69723-94-0	-0.99	-1.528
69770-23-6	2.84	2.691
70124-77-5	6.38	6.869
70343-06-5	1.21	1.320
79124-76-8	2.95	2.964

Compound's Name No CAS Number available	FHM-96 pT Measured	FHM-96 pT Predicted
BAE-7BT; branched alkyl ethoxylate	2.19	2.824
BAE-7PT; branched alkyl ethoxylate	2.01	2.915
LAE-9; linear alkyl ethoxylate	2.69	2.917
12-chlorodehydroabietic acid	2.39	3.223
BNPEO-9; branched nonylphenol (ethoxylate)9	2.14	2.772
cobalt(II) formate	0.67	0.727
lead fluoroborate	1.33	1.323
NEODOL 23-5; linear dodecanol/tridecanol (ethoxylate)5	2.62	2.911
DOBANOL 23-4.5/6; linear dodecanol/tridecanol (ethoxylate)5.25	2.65	2.912
NEODOL 23-6.5; linear dodecanol/tridecanol (ethoxylate)6.5	2.67	2.915
NEODOL 91-6; linear decanol (ethoxylate)6	1.7	2.912
DOBANOL 91-8; linear decanol (ethoxylate)8	1.67	2.916
NEODOL 1-7; linear undecanol (ethoxylate)7	2.09	2.915
NEODOL 1-9; linear undecanol (ethoxylate)9	1.9	2.917
NEODOL 25-12; linear dodecanol/pentadecanol (ethoxylate)12	2.72	2.918
NEODOL 45-13; linear tetradecanol/pentadecanol (ethoxylate)13	2.9	2.918

**Appendix 2**

Number	CAS	Predicted pT	Lower C. pT	Upper C. pT	Predicted mg/L
1		2.54	1.31	3.55	1.03
2		0.78	-0.32	1.92	54
3		-0.05	-1.10	1.14	199
4		1.92	0.73	2.97	3.5
5		2.68	1.43	3.67	0.48
6		1.63	0.47	2.70	3.3
7		1.90	0.71	2.95	2.8
8		3.53	2.21	4.46	0.12
9		4.93	3.51	5.76	0.0041
10		0.44	-0.64	1.60	47
11		1.09	-0.04	2.20	7.9
12		-0.16	-1.20	1.04	113
13		-1.69	-2.61	-0.37	8000
14		3.73	2.40	4.65	0.05
15		0.24	-0.83	1.41	65
16		1.64	0.47	2.71	2.5
17		-0.82	-1.80	0.44	624
18		-0.77	-1.76	0.49	759
19		2.30	1.08	3.32	0.91
20		2.76	1.51	3.75	0.46
21		1.70	0.53	2.77	3.1
22		1.20	0.07	2.31	11
23		1.87	0.68	2.92	2.5
24		1.66	0.49	2.73	3.1
25		1.74	0.57	2.81	3
26		1.74	0.57	2.81	3
27		1.12	-0.01	2.23	16.3
28		0.26	-0.80	1.44	121
29		1.44	0.29	2.53	4.6
30		1.01	-0.11	2.13	12.5
31		1.60	0.43	2.67	3.2
32		0.97	-0.15	2.09	15.2
33		2.03	0.83	3.07	1.5
34		1.75	0.58	2.81	2.9
35		2.52	1.28	3.52	0.65
36		0.48	-0.60	1.64	49
37		-0.37	-1.39	0.85	302
38		-0.18	-1.22	1.02	164
39		2.00	0.80	3.04	2
40		3.35	2.05	4.29	0.12
41		0.75	-0.36	1.88	31
42		0.94	-0.18	2.06	16.1
43		1.62	0.45	2.69	4.6
44		1.20	0.07	2.31	9.9
45		1.14	0.01	2.24	9.2
46		1.49	0.33	2.57	10.2
47		1.01	-0.11	2.13	12.5
48		1.60	0.43	2.67	3.2
49		0.08	-0.98	1.26	77
50		1.10	-0.03	2.21	6.1
51		-0.71	-1.71	0.53	413
52		1.01	-0.11	2.13	12.5
53		1.60	0.43	2.67	3.2
54		2.30	1.08	3.32	0.91
55		0.20	-0.87	1.37	58
56		0.77	-0.34	1.90	27
57		2.19	0.98	3.22	1.3
58		1.94	0.74	2.98	3.3
59		2.79	1.53	3.77	0.37
60		2.58	1.33	3.57	0.65
61		0.33	-0.74	1.50	73

**Appendix 2**

62	2.30	1.08	3.32	0.91
63	2.24	1.02	3.26	0.94
64	-1.18	-2.13	0.11	1730
65	1.19	0.05	2.29	5.7
66	-0.71	-1.71	0.54	485
67	-0.58	-1.58	0.66	627
68	1.29	0.14	2.38	11.7
69	3.92	2.57	4.82	0.035
70	4.26	2.89	5.13	0.017
71	4.13	2.77	5.01	0.022
72	0.90	-0.22	2.02	25
73	1.40	0.25	2.49	3.9
74	1.97	0.77	3.01	2.5
75	1.09	-0.04	2.19	18.9
76	1.35	0.20	2.44	12.7
77	0.33	-0.74	1.50	73
78	1.97	0.77	3.01	1.6
79	0.40	-0.68	1.56	47
80	1.75	0.58	2.81	2.9
81	2.24	1.02	3.26	0.94
82	1.57	0.41	2.64	4.1
83	0.67	-0.42	1.81	36
84	2.52	1.28	3.52	0.65
85	2.19	0.98	3.22	1.1
86	2.83	1.57	3.81	0.54
87	-0.45	-1.47	0.77	446
88	3.60	2.28	4.53	0.08
89	2.78	1.52	3.76	0.41
90	1.68	0.50	2.74	5.6
91	1.99	0.79	3.03	2.4
92	1.80	0.62	2.86	2.3
93	2.17	0.96	3.20	1.3
94	2.77	1.52	3.76	0.44
95	2.68	1.43	3.67	0.48
96	4.27	2.90	5.15	0.019
97	2.43	1.20	3.44	0.78
98	3.04	1.76	4.00	0.41
99	-0.89	-1.87	0.37	904
100	2.44	1.21	3.45	0.65
101				
102	1.54	0.38	2.61	10.2
103	2.30	1.08	3.32	0.91
104	5.49	4.03	6.28	0.0021
105	2.03	0.83	3.07	4
106	1.02	-0.10	2.14	20.3
107	1.22	0.08	2.32	14.5
108	2.68	1.43	3.67	0.48
109	1.97	0.77	3.01	1.6
110	2.67	1.42	3.66	0.46
111	1.85	0.66	2.90	2.8
112	2.67	1.42	3.66	0.46
113	1.84	0.65	2.89	4.8
114	3.37	2.07	4.31	0.16
115	2.68	1.43	3.67	0.48
116	-1.76	-2.68	-0.44	7610
117	1.91	0.72	2.96	2.8
118	2.13	0.92	3.16	2.3
120	0.24	-0.83	1.41	67
121	0.85	-0.26	1.98	36
122	0.62	-0.48	1.76	47
123	-0.15	-1.18	1.06	330
124	1.23	0.09	2.33	13
125	1.46	0.31	2.55	19.4

**Appendix 2**

126				
128	-1.74	-2.66	-0.42	4840
129	0.60	-0.49	1.75	89
130	1.13	0.00	2.24	30
131	0.42	-0.66	1.58	156
132	2.09	0.88	3.12	3
133	-0.06	-1.10	1.14	96
134	0.73	-0.37	1.87	47
135				
136	3.59	2.27	4.51	0.1
137	1.57	0.41	2.64	3.7
138	1.51	0.35	2.59	5.9
139	-0.13	-1.17	1.07	243
141	2.15	0.94	3.18	1.8
142	3.34	2.04	4.29	0.2
143	-0.70	-1.70	0.55	484
144	1.26	0.12	2.35	27
145	1.12	-0.01	2.23	13.5
146	2.42	1.19	3.43	1.3
148	-0.92	-1.90	0.34	1420
149	3.77	2.44	4.68	0.09
150	0.49	-0.60	1.64	168
151	2.30	1.08	3.32	1.1
152	2.50	1.27	3.50	2
153	3.59	2.27	4.51	0.09
155	1.95	0.76	3.00	2.7
157	0.11	-0.95	1.29	61
158	-0.12	-1.16	1.08	122
159	-1.73	-2.65	-0.41	5020
160	0.97	-0.15	2.09	15.2
161	0.97	-0.15	2.09	15.2
162	2.78	1.52	3.76	0.41
163	1.19	0.05	2.29	15
164	2.03	0.83	3.07	1.5
165	0.75	-0.36	1.88	34
166	-0.08	-1.12	1.12	230
167	1.76	0.58	2.82	4
168	1.69	0.51	2.75	3.2
169	1.18	0.04	2.28	11.3
170	1.51	0.35	2.58	6.3
171	1.51	0.35	2.59	12.6
172	1.47	0.31	2.55	9
173	1.48	0.32	2.56	6.1
174	2.23	1.01	3.25	1.3
175	0.24	-0.83	1.41	73
176	0.78	-0.33	1.91	28
177	0.11	-0.95	1.29	61
178	0.61	-0.48	1.76	30
179	0.22	-0.85	1.39	68
180	-0.88	-1.87	0.38	823
181	1.32	0.17	2.41	8.1
182	1.80	0.62	2.86	2.3
183	0.10	-0.95	1.29	59
184	-0.61	-1.61	0.63	442
185	1.03	-0.10	2.14	16.1
186	1.02	-0.10	2.14	15
187	1.03	-0.10	2.14	20.1
188	2.05	0.85	3.09	1.7
189	2.57	1.33	3.57	0.81
190	2.44	1.21	3.45	0.65
191	1.87	0.68	2.92	2.7
192	2.44	1.21	3.45	0.65
193	2.03	0.83	3.07	1.5

**Appendix 2**

194	-0.34	-1.36	0.88	327
195	1.36	0.21	2.45	10.3
196	2.46	1.23	3.47	1.9
197	1.41	0.26	2.50	17.2
198	2.76	1.51	3.75	0.45
199	2.57	1.32	3.56	1.4
200	1.29	0.15	2.39	18.5
201	1.97	0.77	3.01	1.6
202	1.95	0.76	3.00	3
203	1.97	0.77	3.01	1.6
204	1.85	0.66	2.90	3.9
205	2.90	1.64	3.88	0.28
206	1.74	0.56	2.80	9.1
207	1.93	0.74	2.98	4.8
208	1.29	0.15	2.39	21.5
209	2.43	1.20	3.44	1.9
210	2.73	1.47	3.71	0.53
211	2.74	1.48	3.72	0.38
212	1.69	0.52	2.75	9
213	2.09	0.89	3.13	2.6
214	2.23	1.02	3.25	2
215	2.11	0.91	3.15	2.4
216	2.20	0.98	3.22	6.1
217	1.75	0.57	2.81	4.6
218	0.85	-0.26	1.98	40
219	1.37	0.22	2.46	17.7
220	1.02	-0.10	2.14	55
221	3.02	1.74	3.98	0.38
222	2.35	1.13	3.37	1.7
223	3.08	1.80	4.04	0.32
224	1.21	0.07	2.31	40
225	1.42	0.27	2.51	17.1
226	2.52	1.28	3.52	1.3
227	3.30	2.00	4.25	0.15
228	2.03	0.83	3.07	4.3
229	1.53	0.37	2.61	14.6
230	2.19	0.98	3.22	3
231	1.41	0.26	2.50	17.2
232	1.72	0.54	2.78	8
233	3.36	2.06	4.30	0.26
234	1.74	0.56	2.80	7.1
235	3.50	2.19	4.43	0.14
236	2.15	0.95	3.18	5.9
237	1.32	0.17	2.41	19.3
238	1.85	0.66	2.90	6.8
239	2.02	0.82	3.06	6.6
240	1.74	0.56	2.80	7.1
241	2.10	0.89	3.13	3.8
242	1.42	0.26	2.50	18.3
243	2.37	1.14	3.38	2.2
244	2.90	1.63	3.87	0.64
245	1.72	0.54	2.78	7.6
101a	2.62	1.37	3.61	0.78
101b	0.26	-0.80	1.44	120
125a	1.67	0.50	2.74	10
125b	1.28	0.14	2.37	10
126a	2.06	0.86	3.09	1.6
126b	0.33	-0.74	1.50	100
140a	0.35	-0.73	1.51	230
140b	-1.28	-2.23	0.01	1720
150a	0.49	-0.59	1.65	80
150b	-2.15	-3.04	-0.79	21070

**Appendix 2**

Number	SET-2	Predicted [mg/L]	Upper C.L. [mg/L]	Lower C.L. [mg/L]
246		4.76	73.0	0.42
247		91.0	1059	6.12
248		2.35	39.9	0.23
249		12.7	179	1.04
250		67.6	862	4.98
251		20.0	273	1.58
252		10.6	154	0.89
253		17.4	232	1.34
254		63.9	740	4.28
255		62.2	732	4.23
256		51.0	616	3.56
257		23.4	305	1.76
258		33.7	424	2.45
259		1.15	19.9	0.11
260		1.21	20.3	0.12
261		40.6	531	3.07
262		59.6	686	3.97
263		495	4871	28.1
264		81.0	927	5.34
265		159	1700	9.80
266		141	1540	8.88
267		16.6	219	1.26
268		96.7	1100	6.35
269		2.34	37.5	0.22
270		0.28	5.2	0.03
271		0.20	3.9	0.02
272		6.97	101	0.58
273		2.07	33.3	0.19
274		0.89	15.1	0.09
275		198	2168	12.5
276		0.75	12.8	0.07
277		84.7	1008	5.82
278		78.5	946	5.47
279		102	1210	6.99
280		5.48	80.1	0.46
281		0.66	11.3	0.07
282		2.69	42.5	0.25
283		2.20	35.6	0.21
284		6.18	91.6	0.53
285		12.4	167	0.96
286		29.6	375	2.17
287		22.4	283	1.64
288		2.53	39.5	0.23
289		7.11	102	0.59
290		5.48	80.1	0.46
291		10.0	136	0.79
292		5.10	75.4	0.43
293		155	1695	9.78
294		4.82	70.6	0.41
295		2.77	43.2	0.25
296		14.1	191	1.10
297		19.4	253	1.46
298		1.16	19.7	0.11
299		37.5	498	2.88
300		0.36	6.8	0.04
301		182	2147	12.4
302		2.68	42.6	0.25
303		95.1	1121	6.46
304		1.04	17.4	0.10
305		7.11	102	0.59

**Appendix 2**

306	38.7	494	2.85
307	3.57	53.6	0.31
308	9.65	132	0.76
309	9.87	140	0.81
310	9.04	128	0.74
311	7590	62601	359
312	0.57	10.1	0.06
313	4.27	66.1	0.38
314	4.35	67.9	0.39
315	0.76	12.8	0.07
316	0.031	0.68	0.004
317	42.0	538	3.11
318	9.43	138	0.80
319	125	1373	7.92
320	10.9	160	0.92
321	95.3	1158	6.68
322	265	2812	16.3
323	324	3424	19.8
324	5.59	78.3	0.45
325	13.2	194	1.12
326	65.3	746	4.31
327	143	1679	9.71
328	62.2	714	4.13
329	2.05	34.4	0.20
330	113	1276	7.37
331	7.76	114	0.66
332	60.5	713	4.12
333	16.1	204	1.18
334	302	3165	18.3
335	18.9	245	1.41
336	11.6	153	0.88
337	57.6	673	3.89
338	198	2171	12.6
339	10.4	149	0.86
340	25.7	342	1.98
341	1.23	20.5	0.12
342	2.11	34.4	0.20
343	3.31	48.9	0.28
344	1.68	26.7	0.15
345	280	2948	17.0
346	0.048	1.04	0.010
347	107	1187	6.86
348	1098	10383	59.8
349	1.86	30.9	0.18
350	0.51	10.1	0.06
351	11.8	161	0.93
352	32.0	403	2.33
353	99.5	1125	6.51
354	60.8	689	3.97
355	2.31	36.4	0.21
356	0.022	0.50	0.003
357	68.9	852	4.92
358	0.050	1.09	0.010
359	63.7	778	4.50
360	3.72	57.0	0.33
361	7.57	108	0.62
362	8.55	119	0.69
363	68.0	792	4.57
364	399	4176	24.1
365	9.00	134	0.77
366	18.2	231	1.34
367	136	1542	8.89
368	0.49	8.8	0.05

**Appendix 2**

369	0.23	4.4	0.03
370	0.86	14.3	0.08
371	5.11	78.2	0.45
372	862	8414	48.5
373	697	7166	41.3
374	10.0	139	0.81
375	46.3	567	3.28
376	3.28	48.9	0.28
377	415	4197	24.2
378	20.5	268	1.55
379	174	1872	10.8
380	170	1965	11.4
381	18.1	243	1.41
382	16.7	228	1.32
383	26.5	360	2.08
384	1.12	19.6	0.11
385	36.4	453	2.62
386	441	4626	26.7
387	0.73	12.7	0.07
388	0.51	9.1	0.05
389	552	5527	31.9
390	0.84	14.2	0.08
391	0.84	14.2	0.08
392	519	5186	29.9
393	21.0	279	1.62
394	0.17	3.2	0.02
396	577	5840	33.7
397	0.54	9.9	0.06
398	17.8	237	1.37
399	5.35	81.3	0.47
400	40.2	522	3.01
401	21.0	282	1.63
402	38.8	511	2.95
403	2.94	44.1	0.26
404	1122	10924	62.9
405	0.69	12.2	0.07
406	2.01	34.2	0.20
407	1.02	17.0	0.10
408	0.84	14.8	0.09
409	5.03	73.5	0.42
410	3.21	51.0	0.29
411	0.37	6.9	0.04
412	16.2	215	1.24
413	432	4623	26.7
414	0.45	8.4	0.05
415	7.08	106	0.61
416	0.83	14.8	0.09
417	475	4769	27.5
418	418	4300	24.8
419	92.9	1065	6.16
420	1.78	30.8	0.18
421	8.91	125	0.72
422	160	1747	10.1
423	28.7	349	2.02
424	3.47	54.4	0.31
425	15.1	200	1.15
426	3.93	60.2	0.35
427	1.01	16.7	0.10
428	15.6	209	1.21
429	3.85	61.3	0.35
430	16.4	222	1.28
431	1.91	31.8	0.18
432	55.6	671	3.88

**Appendix 2**

433	4.69	73.2	0.42
434	2.83	44.3	0.26
435	1.17	19.8	0.11
436	4.10	61.6	0.36
437	0.027	0.60	0.003
438	3.18	50.0	0.29
439	0.65	11.3	0.07
440	4.83	71.3	0.41
441	0.20	3.8	0.02
442	0.86	14.3	0.08
443	3.47	54.4	0.31
444	7.28	108	0.63
445	247	2790	16.1
446	1.25	21.3	0.12
447	2.56	41.7	0.24
448	0.12	2.3	0.01
449	267	3011	17.4
450	8.76	125	0.72

Number	SET-3	Predicted [mg/L]	Upper C.L. [mg/L]	Lower C.L. [mg/L]
451		0.55	9.75	0.056
452		3.14	47.0	0.27
453		0.66	11.3	0.065
454		4.82	74.8	0.43
455		16.5	232	1.34
456		84.8	1033	5.97
457		10.3	146	0.85
458		0.86	14.3	0.083
459		0.95	16.1	0.093
460		69.2	811	4.68
461		2.42	42.2	0.24
462		3.42	55.8	0.32
463		495	4871	28.1
464		9.72	143	0.83
465		10.8	160	0.93
466		73.4	905	5.23
467		5.5	81.1	0.47
468		0.23	4.40	0.025
469		1.61	26.8	0.16
470		7.14	108	0.62
471		35.6	471	2.73
472		9.17	138	0.80
473		9.21	125	0.72
474		0.03	0.71	0.0040
475		2.93	44.1	0.26
476		2.22	35.7	0.21
477		0.26	5.21	0.030
478		2.96	45.1	0.26
479		37.0	494	2.86
480		280	2948	17.0
481		1.99	33.5	0.19
482		9.85	139	0.80
483		10.4	160	0.93
484		5.29	82.6	0.48
485		7.79	117	0.68
486		10.6	162	0.93
487		5.77	91.7	0.53
488		0.27	5.33	0.031
489		0.96	16.0	0.092
490		3.95	60.2	0.35
491		0.46	8.83	0.051
492		3.8	60.9	0.35

## Appendix 2

493	3.33	53.5	0.31
494	3.37	57.4	0.33
495	1.17	20.6	0.12
496	12.6	189	1.09
497	2.56	40.6	0.23
498	34.2	436	2.52
499	0.68	12.5	0.072
500	9.03	129	0.75
501	4.38	69.3	0.40
502	0.25	5.00	0.029
503	2.54	42.8	0.25
504	1.92	32.0	0.18
505	4.07	65.4	0.38
506	192	2113	12.2
507	56.4	677	3.92
508	87.9	1026	5.93
509	1.41	24.9	0.14
510	2.26	35.3	0.20
511	18.1	252	1.46
512	68.3	812	4.70
513	7.25	114	0.66
514	18.5	243	1.41
515	0.07	1.56	0.0090
516	0.12	2.42	0.014
517	155	1739	10.0
518	1.56	27.3	0.16
519	7.41	105	0.61
520	0.49	8.90	0.051
521	0.15	3.09	0.018
522	9	130	0.75
523	12.6	181	1.05
524	9.21	137	0.79
525	432	4623	26.7
526	3.68	56.6	0.33
527	688	7418	42.8
528	4.99	75.4	0.44
529	12.8	198	1.14
530	1.08	18.3	0.11
531	3.42	52.3	0.30
532	38.4	531	3.07
533	14.1	202	1.17
534	2.13	37.5	0.22
535	0.93	16.5	0.095
536	26.0	359	2.08
537	18.4	261	1.51
538	1.18	20.0	0.12
539	0.99	17.6	0.10
540	1.23	20.7	0.12
541	8.24	123	0.71
542	1.42	25.6	0.15
543	0.97	16.2	0.093
544	1.08	19.7	0.11
545	128	1589	9.19
546	5.22	79.0	0.46
547	33.5	461	2.67
548	4.38	69.4	0.40
549	29.6	423	2.44
550	7.14	114	0.66
551	0.39	7.68	0.044
552	18.5	251	1.45
553	75.5	943	5.45
554	8.32	118	0.68
555	114	1443	8.34

**Appendix 2**

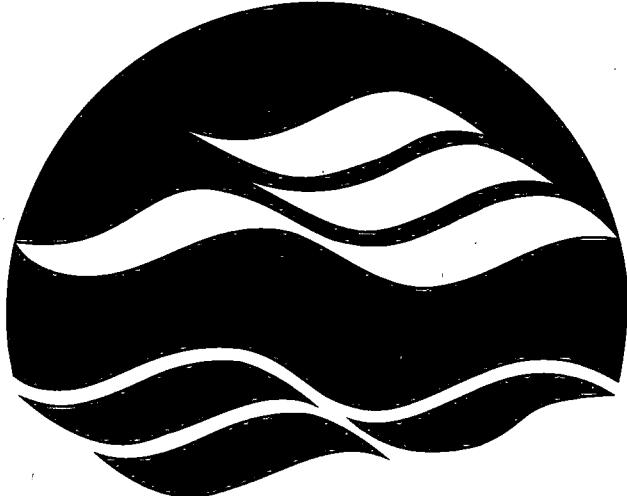
556	62.7	787	4.55
557	107	1374	7.96
558	2401	22558	130
559	1.36	23.6	0.14
560	15.8	225	1.30
561	194	2200	12.7
562	5.51	86.0	0.50
563	39.5	520	3.01
564	0.24	5.06	0.029
565	0.22	4.54	0.026
566	0.21	4.29	0.025
567	0.23	4.80	0.027
568	0.37	6.94	0.040
569	18.8	259	1.50
570	86.3	1057	6.11
571	5.01	79.9	0.46
572	0.70	12.6	0.073
573	36.5	500	2.89
574	9.88	154	0.89
575	11.4	172	0.99
576	50.0	661	3.83
577	21.6	307	1.78
578	39.5	546	3.16
579	49.1	670	3.88
580	4.15	68.2	0.39
581	3.55	59.1	0.34
582	3.14	47.0	0.27
583	1.97	33.3	0.19
584	2.96	50.8	0.29
585	4.05	67.3	0.39
586	1.88	30.7	0.18
587	2.83	46.4	0.27
588	6.09	89.1	0.52
589	6.09	89.1	0.52
590	0.25	5.03	0.029
591	3.39	53.3	0.31
592	10.0	140	0.81
593	3.39	53.3	0.31
594	0.41	7.94	0.046
595	5.99	95.2	0.55
596	2.51	39.7	0.23
597	19.9	266	1.54
598	19.9	266	1.54
599	3.8	63.5	0.37
600	2.56	42.2	0.24
601	2.68	44.4	0.26
602	2.81	46.6	0.27
603	0.25	5.03	0.029
604	0.25	5.03	0.029
605	0.25	5.03	0.029
606	18.7	266	1.54
607	0.54	10.1	0.058
608	173	2086	12.1
609	0.88	16.0	0.092
610	1.12	20.0	0.12
611	9.23	138	0.80
612	28.8	377	2.18
613	96.9	1220	7.06
614	18.5	274	1.58
615	1.58	27.4	0.16
616	5.39	87.0	0.50
617	37.5	472	2.73
618	5.26	82.4	0.48

**Appendix 2**

619	8.19	118	0.68
620	1.48	25.7	0.15
621	6.44	99.3	0.57
622	3.21	49.3	0.29
623	3.21	49.3	0.29
624	23.3	302	1.75
625	20.8	274	1.58
626	1.86	31.6	0.18
627	1.51	25.4	0.15
628	2.59	44.3	0.26
629	2.37	37.1	0.21
630	18.5	259	1.50
631	0.17	3.56	0.020
632	2.14	35.3	0.20
633	17.4	256	1.48
634	1.02	17.9	0.10
635	9.15	146	0.84
636	1.87	32.0	0.18
637	1.22	21.5	0.12
638	148	1844	10.7
639	1.94	33.4	0.19
640	9.73	148	0.85
641	5.28	80.3	0.46
642	0.72	13.4	0.077
643	0.72	13.4	0.077
644	1.23	20.7	0.12
645	38.8	503	2.91
646	8.96	131	0.76
647	20.9	281	1.63
648	4.11	64.6	0.37
649	1550	14622	84.1
248a	15.5	224	1.29
248b	539	5099	29.3
299a	19.2	261	1.51
299b	4528	38434	220
318a	25.3	328	1.90
318b	890	8734	50.3
325a	158	1775	10.2
325b	306	3255	18.8
329a	274	2997	17.3
329b	43.3	552	3.19
395a	2919	25141	144
429a	177	2069	12.0
429b	89.8	1014	5.85
461a	15.5	224	1.29
461b	5584	48485	278
483a	9.19	141	0.81
483b	422	4228	24.3
513a	7.98	123	0.71
513b	422	4228	24.3
515a	0.95	16.6	0.096
515b	539	5099	29.3
527a	18.8	245	1.42
527b	16.2	224	1.29
532a	30.8	428	2.48
532b	422	4228	24.3
533a	18.7	254	1.47
533b	610	6108	35.1
549a	21.8	313	1.81
549b	422	4228	24.3
550a	3.81	63.2	0.37
550b	422	4228	24.3
558a	77.5	875	5.05

**Appendix 2**

<b>558b</b>	<b>23395</b>	<b>178953</b>	<b>1020</b>
<b>562a</b>	<b>6.17</b>	<b>94.9</b>	<b>0.55</b>
<b>562b</b>	<b>519</b>	<b>4820</b>	<b>27.7</b>
<b>587a</b>	<b>0.65</b>	<b>11.8</b>	<b>0.068</b>
<b>587b</b>	<b>1736</b>	<b>15062</b>	<b>86.5</b>
<b>621a</b>	<b>6.1</b>	<b>93.9</b>	<b>0.54</b>
<b>621b</b>	<b>519</b>	<b>4820</b>	<b>27.7</b>
<b>627a</b>	<b>0.92</b>	<b>16.1</b>	<b>0.093</b>
<b>627b</b>	<b>3743</b>	<b>31808</b>	<b>183</b>
<b>649a</b>	<b>645</b>	<b>6229</b>	<b>35.8</b>
<b>649b</b>	<b>76.4</b>	<b>850</b>	<b>4.90</b>



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