Quantitative Structure−Property Relationships for the Estimation of Boiling Point and Flash Point Using a Radial Basis Function Neural Network

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Radial basis function (RBF) neural network models for the simultaneous estimation of flash point (T_f) and boiling point (T_b) based on 25 molecular functional groups and their first-order molecular connectivity index ($^1\chi$) have been developed. The success of the whole modeling process depended on a network optimization strategy based on biharmonic spline interpolation for the selection of an optimum number of RBF neurons (**n**) in the hidden layer and their associated spread parameter (σ). The RBF networks were trained by the Orthogonal Least Squares (OLS) learning algorithm. After dividing the total database of 400 compounds into training (134), validation (133), and testing (133), the average absolute errors obtained for the validation and testing sets ranges from 10 °C to 12 °C and 11 °C to14 °C for T_f and T_b, respectively, and are in agreement with the experimental value of about 10 °C. Results of a standard Partial Least Square (PLS) regression model for single output predictions range from 23 °C to 24 °C and 18 °C to 20 °C for T_f and T_b, respectively, indicating the superior predictive ability of the neural model and strongly suggests that a nonlinear relationship exists between the input and target parameters of the data. The robustness of the neural model was successfully examined by a random split cross validation based on pooling together of the validation and test data sets. The study shows that the simple numerical coding of a molecule based on its formula together with its $^1\chi$ is an attractive way of estimating the flammability properties of organic compounds via an RBF neural network.

INTRODUCTION

In recent years neural networks (NNs) have become an important modeling technique in the field of quantitative structure−activity relationships (QSAR) and/or quantitative structure−property relationships (QSPR). The advantage of NNs is in their inherent ability to incorporate nonlinear and cross product terms into the model. Besides, they do not require a knowledge of the mathematical function to be known in advance. They also enable flexible multiresponse mapping using only one NN model.[1] This flexibility of NNs is especially useful in QSAR/QSPR problems compared to other methods such as multiple linear regression analysis (MLR) or partial least squares (PLS) regression. With MLR, separate modeling equations for each single response have to be developed. While PLS has the capability of multiple response output, prediction performance is sometimes reduced, and, as a result, single output models are preferred in most cases.

The flash point (T_f) is of particular importance since it dictates how a compound may be used, handled, or transported in bulk quantities.[2] It is defined as the temperature at which a material gives off vapor sufficient to form an ignitable mixture with the air near its surface. Empirical correlations between T_f of organic compounds having diverse structures, and their normal boiling points (T_b) have been reported.[3−6] On the other hand, a prediction scheme for flash points of organic compounds from molecular structures based on a QSPR approach was proposed in a previous study.[7] Back-propagation (BP) neural models have been developed to predict T_b and critical temperatures of organic compounds by others.[8,9] Two types of BP networks, gradient descent[10] and the Broyden−Fletcher−Goldfard−Shanno (BFGS)[11] algorithm, were employed in their studies. The modeling process involved the training of over 450 random networks from which the best model was selected. Recently the normal boiling points and critical temperatures have been successfully modeled by BP networks.[12] In all these studies only separate models for the target properties were examined. It is evident from the efforts by Egolf et al.[8,9] and Hall et al.[12] that the inability to explicitly optimize the BP network irrespective of the training algorithm used, necessitated a large number of trial networks from which the best (but not necessarily the optimum network) was selected. The process of obtaining an optimum BP working model is time-consuming indeed, although it does not guarantee the realization of an explicit optimum network configuration. This is due to the random weight initialization used for each model during the start of training. Our previous studies have shown that it is easier and faster to train and optimize RBF neural networks compared to back-propagation networks.[13]

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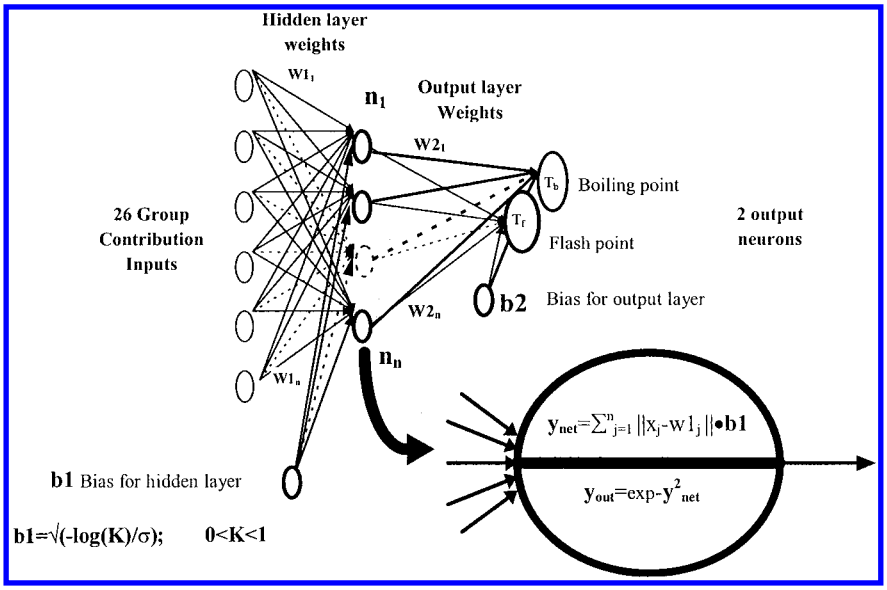

Figure 1. Detailed schematic overview of RBF neural network.

Table 1. Classes of Compounds Used for Modeling T_f and T_b

chemical class	no. samples
aliphatic hydrocarbon	33
aromatic hydrocarbon	26
alcohols	30
phenols	10
ethers	23
aldehydes	10
ketones	17
acids	11
esters	38
nitriles	8
amines and anilines	31
N-containing ring compounds	4
amides and anilides	6
nitro compounds	8
isocyanates	4
thiols	10
sulfides and thiophenes	7
sulfones	2
isothiocyanates	4
halogenated hydrocarbons	35
multifunctional compounds	83

Recently a flexible and robust optimization of RBF neural networks using biharmonic splines has been reported,[14] in which the use of RBF neural networks trained by the orthogonal least squares training (OLS)[15] algorithm enables systematic network optimization by response surface methodology.[11]

In all neural models it is very important to know whether the network has been overtrained. Thus any model built on only a training and test set cannot be confidently considered to be a working model irrespective of the degree of correlation between the predicted and experimental values for the training and validation data sets. An independent set of data not seen directly or indirectly by the model should be used to confirm the true prediction capability of the model. This is the approach used in this report.

The purposes of the present study are to show the flexible modeling capabilities of RBF neural networks explicitly optimized by a spline response surface to develop a single RBF model capable of simultaneous prediction of T_f and T_b for a nonhomogeneous functional group database and to compare the results with a factor based multivariate linear regression systems such as PLS.[16,17]

Table 2. Input Parameters for 2-Chlorobenzotrifluororide[a]

	name	2-chlorobenzotrifluoride
	formula	$C_7H_4ClF_3$
boiling point	T_b	152.2
flash point	T_f	59.0
	Descriptor	input value
1	$^1\chi$	5.183
2	C_{ar}	6
3	OH_{al}	0
4	OH_{ph}	0
5	−O−	0
6	CHO	0
7	CO	0
8	COOH	0
9	−COO−	0
10	CN	0
11	SH	0
12	−S−	0
13	NO2	0
14	NH2	0
15	NH	0
16	N_{al}	0
17	N_{ar}	0
18	F	3
19	Cl	1
20	Br	0
21	I	0
22	CONH	0
23	CON	0
24	−SO2−	0
25	NCS	0
26	NCO	0

[a] Subscripts: $_{ar}$ = aromatic, $_{al}$ = aliphatic, $_{ph}$ = phenols.

OVERVIEW OF RBF NETWORKS

The theory of RBF networks has been extensively presented in the literature[18−20] so a basic overview is presented here. Figure 1 shows a detailed network architecture of the RBF neural network with a Gaussian function hidden layer neuron. The input layer **x** consists of the descriptors (26 inputs were used in this paper), and the two target outputs are T_f and T_b. The goal is to generate weights, **w**, and bias, **b**, connected between the input and hidden layer neuron **n**, and between the hidden layer neurons to the output targets. The method of learning, that is the generation of the appropriate **w** and **b**, determines how quickly the final model

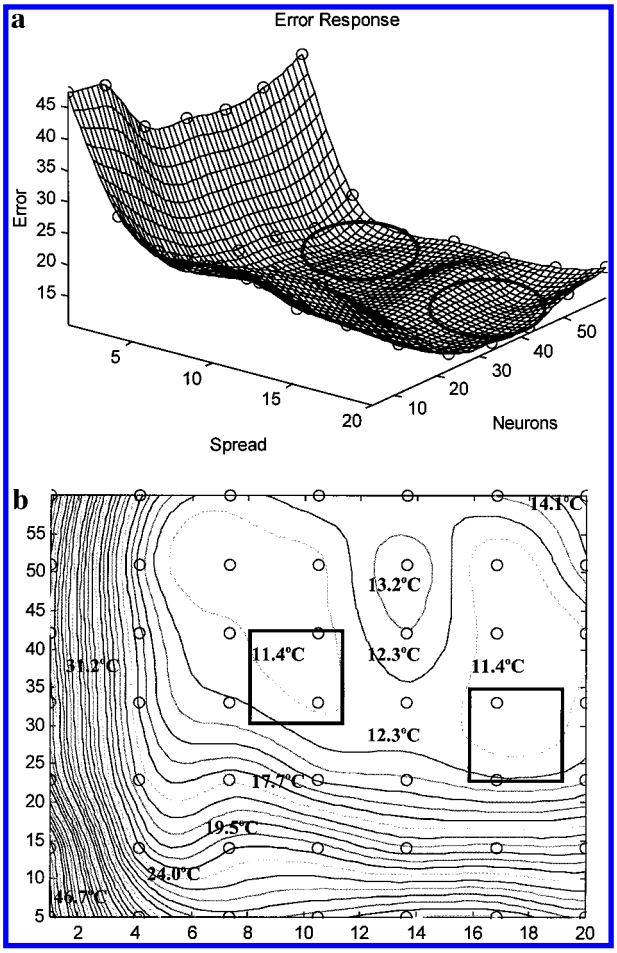

Figure 2. Error response surface (a) 3D view and (b) contour view, used for locating optimum RBF network configuration generated by the biharmonic spline interpolation for the simultaneous prediction of T_f and T_b.

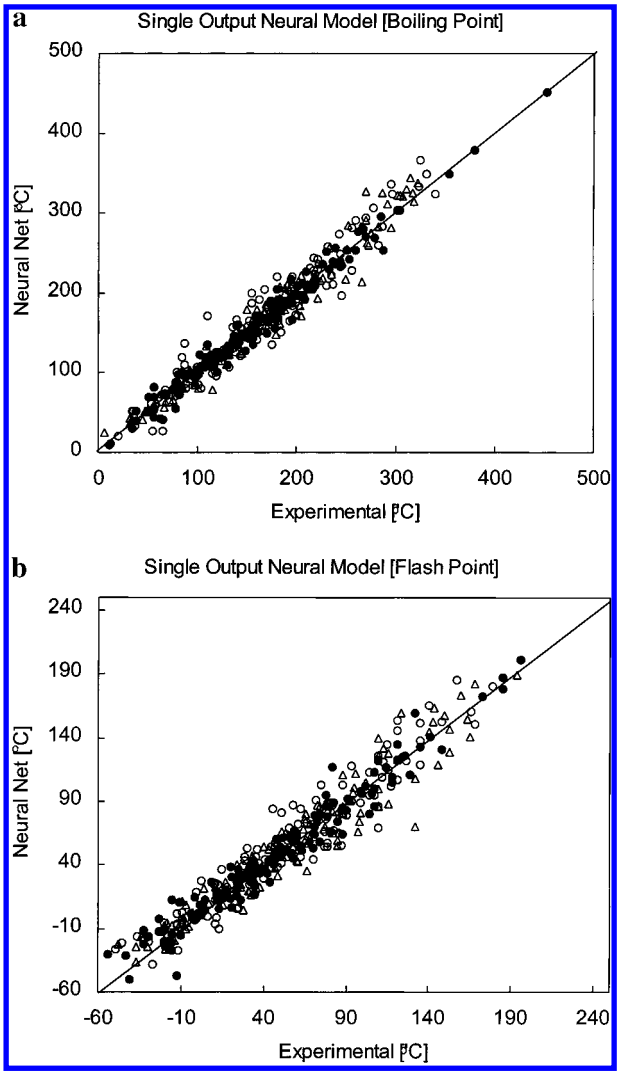

Figure 3. Single output RBF prediction**. (a) T_b (●) training σ = 16.5, **n** = 36, n = 135, r = 0.9891, AE = 8.5 °C, SE = 11.4 °C, (△) validation n = 133, r = 0.9810, AE = 11.1 °C, SE = 15.1 °C, (○) testing n = 130, r = 0.9660, AE = 14.7 °C, SE = 19.4 °C. (b) T_f (●) training σ = 16.8, **n** = 26, n = 135, r = 0.9774, AE = 8.0 °C, SE = 10.8 °C, (△) validation n = 133, r = 0.9629, AE = 10.6 °C, SE = 14.1 °C, (○) testing n = 132, r = 0.9568, AE = 11.9 °C, SE = 14.3 °C.

is obtained and also its prediction ability. In generating neural models, the task of the analyst is to determine the optimum number of neurons **n** in the hidden layer and the appropriate spread or scaling parameter σ capable of predicting the target with minimum error. The generalized network configuration may be represented by **[X**−n_σ**-Y]** where **X** is the input and **Y** is the target.

Several schemes have been proposed to determine **w**, normally called the centriod of the RBF function, and σ, the spread parameter of the Gaussian function. Lowe[21] for example proposed a way to determine the centers based on standard deviations of the training data. Moody and Darken[22] on the other hand selected the centers by means of data clustering techniques that assume that similar input vectors produce similar outputs; σ is then obtained by heuristically taking the average distance to several nearest neighbors of the centers. Other schemes have also been reported including generalization properties[23] and sequential adaptation.[24] In this work we adopted the Orthogonal Least Squares (OLS) training algorithm developed by Chen et al. The OLS requires the fixing of σ during training, and we have developed a simultaneous optimization of **n** and σ around this algorithm, described in detail else where.[15,25] Using this strategy, a fast and explicit optimization of a RBF network can be obtained. A summary of the functional relationships between **x**, **w**, **n**, **b**, and σ are presented in Figure 1. A summary of the algorithm is presented below.

The network receives as net input the vector distance ||**x**−**w**|| between the weight vector **w** and the input vector **x** multiplied by the bias **b**. The bias is a direct function of the spread parameter σ which determines the proportion of input space where the jth RBF neuron has sufficient nonzero response. Thus the spread should be of such a value that neurons respond strongly to overlapping regions of the input space. During training, neurons are created one at a time. At each iteration (i.e. addition of a neuron to the hidden layer which is different from weight adjustments in back-propagation), the input vector which will result in lowering the network error the most is used to create a RBF neuron. The error of the network is checked, and if lower than the set sum of squared errors, training is terminated. Otherwise the next neuron is added. This procedure is repeated until the error level set is met or the set maximum neuron is reached.

This training algorithm is different from the approach where initial weights are randomly generated and training requires simultaneous weight adjustments in the hidden and output layers during each iteration to achieve error minimiza-

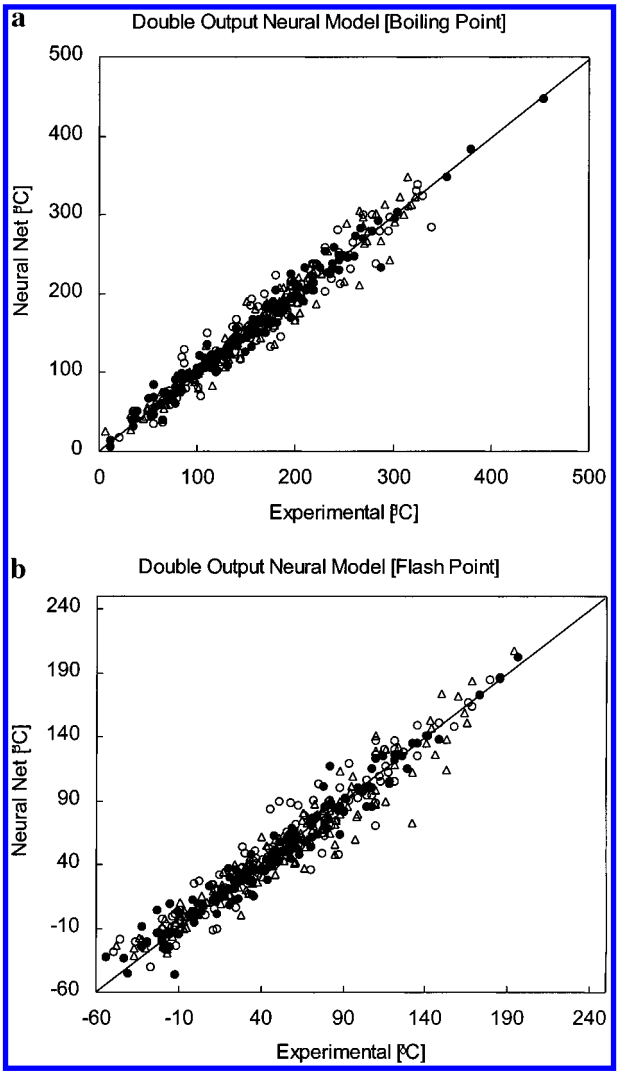

Figure 4. Double output RBF prediction**. (a) T_b (●) training σ = 16.5, **n** = 36, n = 135, r = 0.9879, AE = 8.7 °C, SE = 12.0 °C, (△) validation n = 133, r = 0.9781, AE = 11.0 °C, SE = 15.6 °C, (○) testing n = 130, r = 0.9674, AE = 13.5 °C, SE = 17.8 °C. (b) T_f (●) training σ = 16.5, **n** = 36, n = 135, r = 0.9805, AE = 7.2 °C, SE = 10.1 °C, (△) validation n = 133, r = 0.9632, AE = 10.6 °C, SE = 14.6 °C, (○) testing n = 132, r = 0.9602, AE = 10.8 °C, SE = 14.0 °C.

tion. In this scheme, there is no need to adjust the 1008 *weight* parameters in the 26−36−2 network (i.e. 26 × 36 + 36 × 2) for each iteration. In fact only 36 calculations equivalent to the number of RBF hidden layer neurons are required for a 26−36−2 RBF network configuration. This enables very fast training compared to the traditional iterative schemes, yet the algorithm is numerically stable.

EXPERIMENTAL SECTION

Data Preparation. The T_b and T_f values of 400 compounds were collected from the literature[26,27] and used for this study. The functional groups represented by this data set are shown in Table 1. Each molecule is described by 25 structural properties easily represented in a vector of elements by means of the SMILES (Simplified Molecular Input Lines System) notation.[28] An additional descriptor, the molecular connectivity index[29] $^1\chi$, was included to make a final total of 26 elements in the input vector. Where the functionalities do not apply the value zero is used. For example the input values for 2-chlorobenzotrifluororide are presented in Table 2 to show the diversity of functionalities used to describe each molecule.

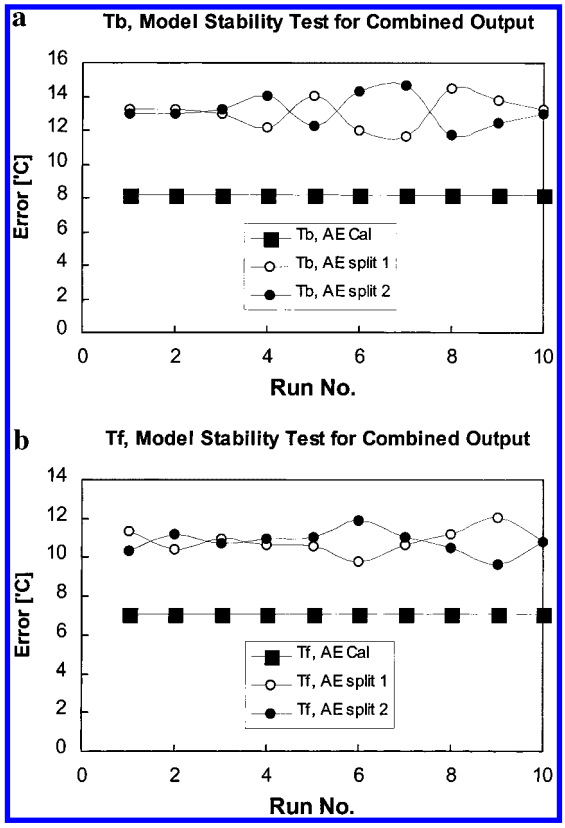

Figure 5. Random split cross validation test for model stability and performance for double output prediction. (a) T_b and (b) T_f.

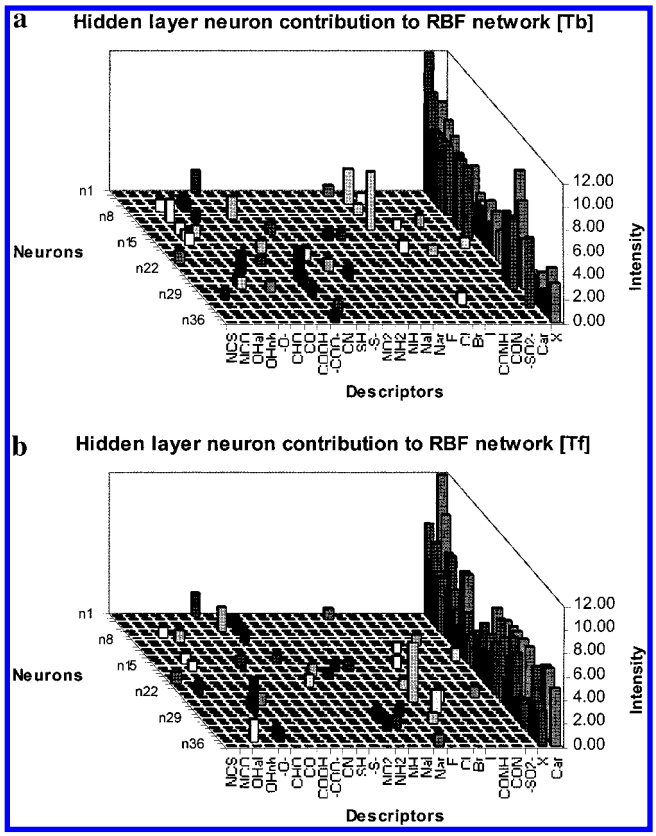

Figure 6. Hidden layer weight distribution for single output (a) T_b and (b) T_f.

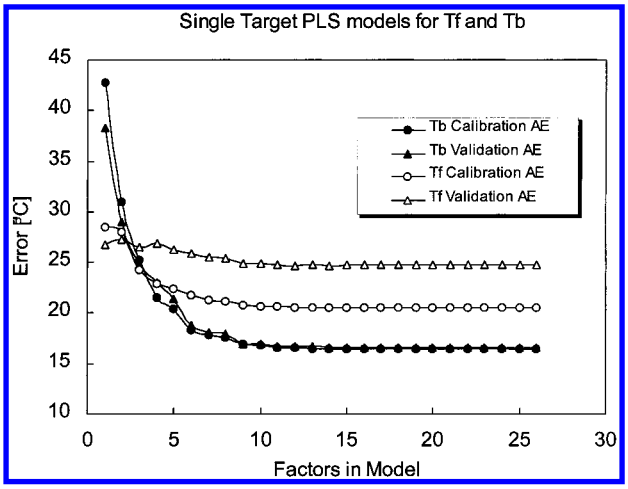

Figure 7. PLS factor selection versus error profile for **single** output models.

Table 3. Summary of Average Absolute Error (AE)* Profiles for the Different Modeling Configuration

(a) RBF Single Output Prediction Errors

	training	validation	testing
T_b/°C	8.5	11.1	14.7
T_f/°C	8.0	10.6	11.9

(b) RBF Double Output Prediction Errors

	training	validation	testing
T_b/°C	8.2	11.4	14.8
T_f/°C	7.1	10.5	11.2

(c) PLS Single Output Prediction Errors

	training	validation	testing
T_b/°C	16.8	16.6	18.4
T_f/°C	20.6	24.7	23.3

(d) PLS Double Output Prediction Errors

	training	validation	testing
T_b/°C	16.8	17.4	19.1
T_f/°C	20.9	24.8	23.8

The choice of input parameters was based on findings in previous report[30] exploring the quantitative relationship between chemical structure and T_f. A principal component analysis (PCA) was performed on a data set of 50 organic compounds and 10 other physical properties. It was determined that only two structural factors were found to satisfactorily reproduce the T_f data. The first is related to the bulk, i.e., size and shape of the molecule which is closely correlated with its $^1\chi$. The second significant factor is related to the specific polar characteristics of the functional groups in the molecule and can be correlated directly with structural additivity scheme. Thus the $^1\chi$ and 25 atomic or group increments were identified to be significant parameters for prediction T_f of organic compounds having diverse structures.[7]

A database of 400 compounds was considered large enough to perform independent training, validation, and testing instead of the leave *part* out cross-validation strategy used when data is very limited. To generate data for training, validation, and prediction, a coding system was used. The whole data set was grouped according to their main functionalities, alkanes, alkene, etc., and numbered from 1 to 400. Beginning from compound number 1, a numbering system

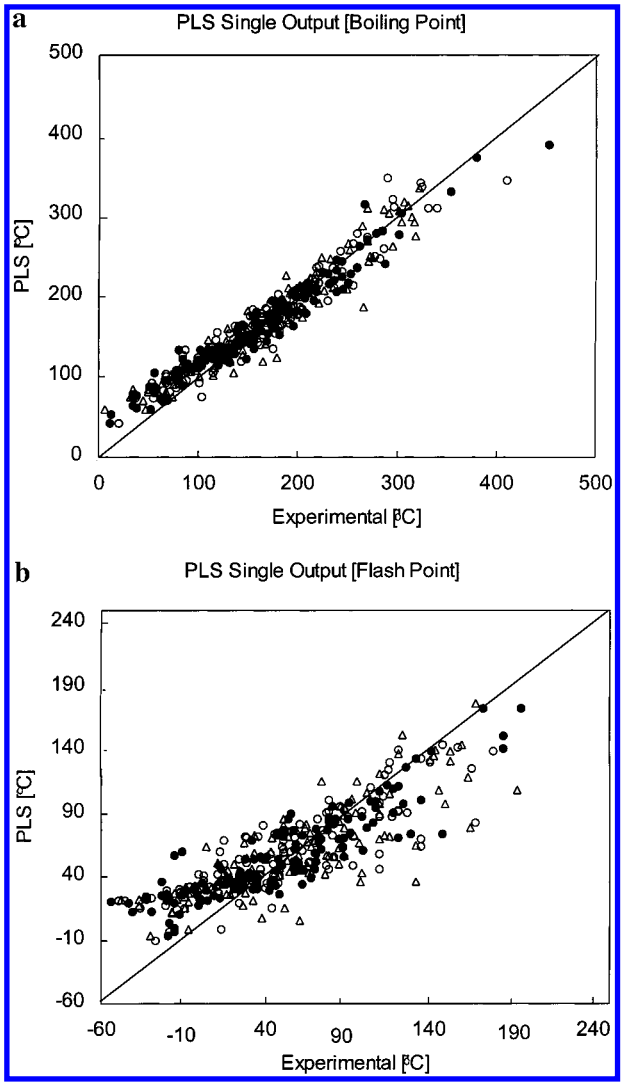

Figure 8. PLS prediction of (a) T_b and (b) T_f.

from 1 to 3 was used and repeated until each compound has a 1, 2, or 3 as an identity code. The whole data was then sorted so that all compounds with similar codes were grouped together. This resulted in 134(code1), 133(code2), and 133-(code3) molecules listed in Tables 4−6, respectively. All the subset data coded 1 were used to build the model. The subset of data coded 2 were used to validate the model, and the final subset coded 3 was used to test the model when the optimum network configuration has been found from subsets 1 and 2. Software used for both neural networks and PLS was developed in the Matlab[31] environment running on a 166 MHz PC. No pretreatment of data such as mean-centering or variance scaling was performed for both neural and PLS models since such treatment results in prediction deterioration for this type of QSPR data. A typical training and optimization session for neural networks and PLS takes less than 10 min.

Training and Optimization. The biharmonic optimization strategy is essentially a response surface analysis with the x, y, z coordinates being **n**, σ, and **Error**, respectively, where the error (z) is the surface to be analyzed. Taking advantage of the convergence stability and the training speed of the OLS algorithm, key networks at (**n**, σ) and their corresponding errors were generated. A response surface obtained from

Table 4. (a) Input Parameters for Training/Calibration Data Set and (b) Output Results for Training/Calibration Data Sets

		Descriptors																										
Training Inputs																												
No. Compound [CAS No]	Comp No.	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO
1. Isoprene [78-79-5]	1	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4. 1,4-Hexadiene [592-45-0]	4	**2.914**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
7. Hexane [110-54-3]	7	2.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10. Methylcyclohexane [108-87-2]	10	3.394	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13. 4-Vinyl-1-cyclohexene [100-40-3]	13	3.932	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16. Ethylcyclohexane [1678-91-7]	16	3.932	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19. Nonane [111-84-2]	19	4.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22. cis-Decalin [493-01-6]	22	4.966	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25. Dodecane [112-40-3]	25	5.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28. Tetradecane [629-59-4]	28	6.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31. Heptadecane [629-78-7]	31	8.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34. Benzene [71-43-2]	34	3	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37. o-Xylene [95-47-6]	37	3.972	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40. m-Vinyltoluene [100-80-1]	40	4.326	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43. Propylbenzene [103-65-1]	43	4.432	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46. Tetralin [119-64-2]	46	4.966	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49. o-Diethylbenzene [135-01-3]	49	4.88	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52. sec-Butylbenzene [135-98-8]	52	4.843	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55. 1-Phenylhexane [1077-16-3]	55	5.932	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58. 1-Phenyloctane [2189-60-8]	58	6.932	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61. Ethanol [64-17-5]	61	1.414	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64. 2-Propanol [67-63-0]	64	1.732	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67. 2-Methyl-2-propen-1-ol [513-42-8]	67	2.27	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70. Isobutyl alcohol [78-83-1]	70	2.27	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73. 2,2-Dimethyl-1-propanol [75-84-3]	73	2.561	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76. t-Amyl alcohol [75-85-4]	76	2.56	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
79. 2-Hexanol [626-93-7]	79	3.27	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82. 1-Heptanol [111-70-6]	82	3.914	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86. 2-Octanol [123-96-6]	85	4.27	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88. 1-Decanol [112-30-1]	**88**	**5.44**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
91. o-Cresol [95-48-7]	91	3.805	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94. 4-Ethylphenol [123-07-9]	94	4.326	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97. p-t-Butyl-o-cresol [98-27-1]	**97**	**5.41**	**6**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
100. Dimethyl ether [115-10-6]	100	1.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
103. 2,2-Dimethyloxirane [3266-23-7]	103	2.207	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106. Methyl propyl ether [557-17-5]	106	2.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109. Isopropyl vinyl ether [926-65-8]	109	2.77	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112. Dipropyl ether [111-43-3]	112	3.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115. Phenetole [103-73-1]	115	4.432	6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118. Methyl p-t-pentylphenyl ether[2050-03	118	6.098	6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
121. Butyl p-t-pentylphenyl ether	121	7.598	6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
124. 2-Propenal [107-02-8]	124	1.914	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
127. Methacrolein [78-85-3]	127	2.27	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
130. Benzaldehyde [100-52-7]	130	3.932	6	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
133. Acetone [67-64-1]	133	1.732	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
136. Cyclopentanone [120-92-3]	136	2.894	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
139. Cyclohexanone [108-94-1]	139	3.394	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
142. 4-Methyl-2-pentanone [108-10-1]	142	3.126	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
145. 5-Methyl-2-hexanone [110-12-3]	145	3.626	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
148. 2-Nonanone [821-55-6]	148	4.77	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
151. Acrylic acid [79-10-7]	151	2.27	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
154. Isobutyric acid [79-31-2]	154	2.643	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
157. 2-Methylvaleric acid [97-61-0]	157	3.681	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
161. Methyl formate [107-31-3]	**160**	**4.77**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
163. Methyl acetate [79-20-9]	163	2.27	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
166. Ethyl acetate [141-78-6]	166	2.77	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
169. Methyl propionate [554-12-1]	169	2.808	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
172. Butyl formate [592-84-7]	172	3.414	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
175. Isopropyl acetate [108-21-4]	175	3.126	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
178. Butyl acetate [123-86-4]	178	3.77	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
181. Ethyl butyrate [105-54-4]	181	3.808	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
184. Isopentyl acetate [123-92-2]	184	4.126	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
187. Phenyl acetate [122-79-2]	187	4.788	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
190. Isobutyl butyrate [539-90-2]	190	4.664	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
193. Isopentyl butyrate [106-27-4]	193	5.164	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
196. 2-Ethylhexyl acetate [103-09-3]	196	5.702	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
199. Acrylonitrile [107-13-1]	199	1.914	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
202. Cyclopropanecarbonitrile [5500-21-0]	202	2.808	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
205. Hexanenitrile [628-73-9]	205	3.414	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
208. Allylamine [107-11-9]	208	1.914	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
211. Butylamine [109-73-9]	211	2.414	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
214. Diethylamine [109-89-7]	214	2.414	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
217. Pentylamine [110-58-7]	**217**	**2.914**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
220. Hexylamine [111-26-2]	220	3.414	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
223. 1,3-Dimethylbutylamine [108-09-8]	223	3.126	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
226. Heptylamine [111-68-2]	226	3.914	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
229. Octylamine [111-86-4]	229	4.414	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
232. N,N-Diethylaniline [91-66-7]	232	5.381	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
235. p-t-Pentylaniline [2049-92-5]	235	5.56	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
238. Pyridine [110-86-1]	238	3	5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
241. Quinoline [91-22-5]	241	4.966	9	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
244. Acetoanilide [103-84-4]	244	4.787	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
247. N-Butylacetanilide [91-49-6]	247	6.753	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
250. 2-Nitropropane [79-46-9]	250	2.643	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
253. m-Nitrotoluene [99-08-1]	253	4.698	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
256. Methyl isocyanate [624-83-9]	256	1.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
259. Cyclohexyl isocyanate [3173-53-3]	259	4.432	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
262. 1-Butanethiol [109-79-5]	262	2.414	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
265. 1-Hexanethiol [111-31-9]	265	3.414	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
268. 1-Octanethiol [111-88-6]	268	4.414	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
271. Thiophene [110-02-1]	271	2.5	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
274. Diallyl sulfide [592-88-1]	**274**	**3.414**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
277. Dipropyl sulfone [598-03-8]	277	4.121	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
280. Allyl isothiocyanate [57-06-7]	280	2.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
283. Ethyl chloride [75-00-3]	283	1.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
286. Isopropyl chloride [75-29-6]	286	1.732	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
289. 1-Bromobutane [109-65-9]	289	2.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
292. 2-Fluoro-2-methylpropane [353-61-7]	292	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
295. 1-Bromopentane [110-53-2]	295	2.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
298. Fluorobenzene [462-06-6]	**298**	**3.394**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
301. 1-Bromohexane [111-25-1]	**301**	**3.414**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
304. o-Bromotoluene [95-46-5]	304	3.805	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
307. m-Chlorotoluene [108-41-8]	307	3.788	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
310. 2-Iodotoluene [615-37-2]	310	3.805	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0

Table 4. (Continued)

Training Inputs (Descriptors)																											
No. Compound [CAS No]	Comp No.	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO
313. 1-Iodoheptane [4282-40-0]	313	3.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
316. 1-Chlorooctane [111-85-3]	316	4.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
319. Acetyl chloride [75-36-5]	319	1.732	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
322. N,N-Dimethylhydrazine [57-14-7]	322	1.732	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0
325. 2-Chloropropionic acid [598-78-7]	325	2.643	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
328. Propyl nitrate [627-13-4]	328	3.27	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
331. 2-(Methylamino)ethanol [109-83-1]	331	2.414	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
334. Ethyl bromoacetate [105-36-2]	334	3.308	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
337. Acetone cyanohydrin [75-86-5]	337	2.581	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
340. 1,4-Thioxane [15980-15-1]	340	3	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
343. 1,2-Dimethoxyethane [110-71-4]	343	2.914	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
346. Diethylene glycol [111-46-6]	346	3.414	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
349. 2-(2-Aminoethylamino)ethanol[111-41-1]	349	3.414	0	1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
352. 2,4-Pentanedione [123-54-6]	352	3.126	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
355. 3-Ethoxypropionic acid [4324-38-3]	355	3.77	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
358. Bromopentafluorobenzene [344-04-7]	358	5.484	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	1	0	0	0	0	0	0
361. 2,4-Dichlorophenol [120-83-2]	361	4.198	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
364. Ethyl acetoacetate [141-97-9]	364	4.164	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
366. Adipic acid [124-04-9]	366	4.626	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
367. Ethylene glycol diacetate [111-55-7]	367	4.626	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
370. 2-Ethoxyethyl acetate [111-15-9]	370	4.27	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
373. 1,2-Diethoxyethane [629-14-4]	373	3.914	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
376. 2-Chlorobenzotrifluororide [88-16-4	376	5.163	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	0	0	0	0	0	0	0
379. Salicylaldehyde [90-02-8]	379	4.343	6	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
382. Phenacyl chloride [532-27-4]	382	4.843	6	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
385. 2-Phenoxyethanol [122-99-6]	385	4.932	6	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
388. Bis[2-(2-chloroethoxy)ethyl] ether [638-556-2]	388	6.414	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
391. Dibutoxymethane [2568-90-3]	391	5.414	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
394. Pentyl salicylate [2050-08-0]	394	7.253	6	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
397. Anthraquinone [84-65-1]	397	7.788	12	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
400. Ethyl(o-(ethoxycarbonyl)-benzoyloxyacetate) [84-72-0]	400	9.896	6	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Training (Target & Results)			Experimental Data		ANN Predictions: Combined Model		ANN Predictions: Single output		PLS Predictions: Single Output	
No. Compound [CAS No]	Formula	Comp No.	Tb	Tf	Tb	Tf	Tb	Tf	Tb	Tf
1. Isoprene [78-79-5]	C5H8	1	34.1	-54.0	40.2	-32.5	37.8	-30.49	74.6	20.0
4. 1,4-Hexadiene [592-45-0]	C6H10	4	66.1	-21.1	73.1	-13.4	72.9	-12.31	95.8	25.6
7. Hexane [110-54-3]	C6H14	7	68.7	-23.0	73.1	-13.4	72.9	-12.31	95.8	25.6
10. Methylcyclohexane [108-87-2]	C7H14	10	101.1	-4.0	96.8	0.6	97.0	1.24	111.6	29.9
13. 4-Vinyl-1-cyclohexene [100-40-3]	C8H12	13	128.0	16.1	122.4	16.1	122.3	16.35	129.2	34.6
16. Ethylcyclohexane [1678-91-7]	C8H16	16	132.0	35.0	122.4	16.1	122.3	16.35	129.2	34.6
19. Nonane [111-84-2]	C9H20	19	150.8	31.0	144.5	29.9	143.6	29.77	145.1	38.8
22. cis-Decalin [493-01-6]	C10H18	22	195.8	58.0	168.9	45.5	166.7	44.94	163.2	43.7
25. Dodecane [112-40-3]	C12H26	25	216.3	71.0	208.1	71.7	204.3	70.27	194.4	52.0
28. Tetradecane [629-59-4]	C14H30	28	253.6	100.0	245.9	98.7	242.8	95.67	227.3	60.8
31. Heptadecane [629-78-7]	C17H36	31	302.2	148.0	295.9	138.0	303.3	130.38	276.6	74.0
34. Benzene [71-43-2]	C6H6	34	80.1	-11.0	93.8	3.7	97.0	10.90	133.6	60.2
37. o-Xylene [95-47-6]	C8H10	37	144.4	32.0	144.1	32.9	148.8	37.67	165.6	68.7
40. m-Vinyltoluene [100-80-1]	C9H10	40	172.2	51.0	161.4	43.2	166.0	47.25	177.2	71.8
43. Propylbenzene [103-65-1]	C9H12	43	159.2	47.0	166.5	46.3	171.0	50.09	180.7	72.8
46. Tetralin [119-64-2]	C10H12	46	207.6	71.0	191.5	61.6	195.3	64.24	198.2	77.5
49. o-Diethylbenzene [135-01-3]	C10H14	49	183.3	57.2	187.6	59.1	191.5	61.98	195.4	76.7
52. sec-Butylbenzene [135-98-8]	C10H14	52	173.4	52.0	185.9	58.1	189.8	61.01	194.2	76.4
55. 1-Phenylhexane [1077-16-3]	C12H18	55	226.0	83.0	233.6	88.3	236.2	88.86	230.0	86.0
58. 1-Phenyloctane [2189-60-8]	C14H22	58	262.0	107.0	273.0	114.9	276.5	112.74	262.9	94.8
61. Ethanol [64-17-5]	C2H6O	61	78.3	13.0	60.2	1.2	54.6	5.46	96.3	45.9
64. 2-Propanol [67-63-0]	C3H8O	64	82.4	12.0	77.5	10.9	74.5	14.42	106.7	48.7
67. 2-Methyl-2-propen-1-ol [513-42-8]	C4H8O	67	113.9	33.3	106.1	27.2	106.2	29.61	124.4	53.4
70. Isobutyl alcohol [78-83-1]	C4H10O	70	108.0	28.0	106.1	27.2	106.2	29.61	124.4	53.4
73. 2,2-Dimethyl-1-propanol [75-84-3]	C5H12O	73	113.5	37.0	121.2	35.8	122.3	37.62	134.0	56.0
76. t-Amyl alcohol [75-85-4]	C5H12O	76	102.3	41.0	121.1	35.6	122.2	37.60	134.0	56.0
79. 2-Hexanol [626-93-7]	C6H14O	79	139.8	57.8	156.7	56.7	158.7	57.76	157.3	62.2
82. 1-Heptanol [111-70-6]	C7H16O	82	175.8	73.0	187.4	75.2	186.6	75.65	178.5	67.9
86. 2-Octanol [123-96-6]	C8H18O	85	180.0	87.8	203.7	85.3	204.1	85.41	190.2	71.0
88. 1-Decanol [112-30-1]	C10H22O	88	230.2	82.0	253.8	117.5	250.9	116.56	228.8	81.3
91. o-Cresol [95-48-7]	C7H8O	91	191.0	81.0	189.2	75.5	184.9	65.79	188.4	95.2
94. 4-Ethylphenol [123-07-9]	C8H10O	94	219.0	103.9	204.9	85.1	208.8	80.16	205.5	99.8
97. p-t-Butyl-o-cresol [98-27-1]	C11H16O	97	287.5	117.8	233.4	103.9	252.7	108.99	241.1	109.3
100. Dimethyl ether [115-10-6]	C2H6O	100	-24.9	-41.0	-0.8	-45.3	-4.2	-49.68	43.5	12.7
103. 2,2-Dimethyloxirane [3266-23-7]	C4H8O	103	65.0	-15.0	40.3	-23.9	40.7	-27.47	69.8	19.7
106. Methyl propyl ether [557-17-5]	C4H10O	106	38.9	-20.0	50.8	-18.3	51.5	-21.64	76.4	21.5
109. Isopropyl vinyl ether [926-65-8]	C5H10O	109	56.0	-32.0	68.4	-8.9	69.5	-11.59	88.1	24.6
112. Dipropyl ether [111-43-3]	C6H14O	112	90.6	21.1	99.4	8.0	99.7	6.56	109.3	30.3
115. Phenetole [103-73-1]	C8H10O	115	170.0	62.8	166.7	59.9	168.4	55.22	177.7	73.0
118. Methyl p-t-pentylphenyl ether[2050-03	-5] C12H18O	118	238.9	98.9	237.9	100.8	236.3	97.94	232.5	87.7
121. Butyl p-t-pentylphenyl ether	C15H24O	121	285.0	135.0	292.2	135.2	295.2	132.34	281.8	100.9
124. 2-Propenal [107-02-8]	C3H4O	124	52.7	-18.9	44.9	-25.2	51.4	-24.08	59.6	-6.3
127. Methacrolein [78-85-3]	C4H6O	127	69.0	-15.0	63.6	-14.6	71.8	-14.08	71.3	-3.1
130. Benzaldehyde [100-52-7]	C7H6O	130	178.0	63.0	163.0	47.8	155.1	51.31	160.9	45.3
133. Acetone [67-64-1]	C3H6O	133	56.3	-20.0	47.2	-20.7	44.3	-20.00	80.5	22.4
136. Cyclopentanone [120-92-3]	C5H8O	136	130.7	26.0	107.9	13.8	110.3	12.64	118.7	32.7
139. Cyclohexanone [108-94-1]	C6H10O	139	156.0	44.0	132.6	28.3	135.5	26.65	135.2	37.1
142. 4-Methyl-2-pentanone [108-10-1]	C6H12O	142	116.7	18.0	119.5	20.5	122.2	19.15	126.3	34.7
145. 5-Methyl-2-hexanone [110-12-3]	C7H14O	145	145.6	36.0	143.8	35.0	146.5	33.13	142.8	39.1
148. 2-Nonanone [821-55-6]	C9H18O	148	195.3	80.0	196.2	87.2	196.7	84.58	180.4	49.2
151. Acrylic acid [79-10-7]	C3H4O2	151	140.5	54.0	137.2	49.8	135.0	51.80	163.6	85.8
154. Isobutyric acid [79-31-2]	C4H8O2	154	154.5	55.6	156.8	61.2	156.0	62.63	175.8	89.1
157. 2-Methylvaleric acid [97-61-0]	C6H12O2	157	200.5	91.1	208.6	92.1	208.9	92.45	210.0	98.2
161. Methyl formate [107-31-3]	C2H4O2	160	239.3	110.0	258.5	123.3	256.9	122.82	245.8	107.8
163. Methyl acetate [79-20-9]	C3H6O2	163	56.3	-10.0	46.9	-14.1	54.4	-15.70	87.4	27.6
166. Ethyl acetate [141-78-6]	C4H8O2	166	77.1	-3.0	73.5	-0.4	79.4	-1.58	103.9	32.0
169. Methyl propionate [554-12-1]	C4H8O2	169	79.7	-2.0	75.5	0.6	81.2	-0.51	105.1	32.3
172. Butyl formate [592-84-7]	C5H10O2	172	106.8	18.0	106.8	17.0	109.0	16.58	125.1	37.6
175. Isopropyl acetate [108-21-4]	C5H10O2	175	89.5	2.0	92.1	9.2	96.1	8.47	115.6	35.1
178. Butyl acetate [123-86-4]	C6H12O2	178	126.1	24.0	124.6	26.4	124.3	26.57	136.8	40.8
181. Ethyl butyrate [105-54-4]	C6H12O2	181	121.6	24.0	126.5	27.4	125.9	27.63	138.0	41.1
184. Isopentyl acetate [123-92-2]	C7H14O2	184	142.0	25.0	142.0	35.8	138.9	36.50	148.5	43.9
187. Phenyl acetate [122-79-2]	C8H8O2	187	195.7	80.0	193.9	69.1	186.9	66.09	205.2	83.5
190. Isobutyl butyrate [539-90-2]	C8H16O2	190	157.2	50.0	167.6	49.8	160.0	51.35	166.1	48.6
193. Isopentyl butyrate [106-27-4]	C9H18O2	193	177.8	59.0	190.4	62.6	178.8	64.92	182.6	53.0
196. 2-Ethylhexyl acetate [103-09-3]	C10H20O2	196	198.0	71.0	214.1	76.2	198.3	79.21	200.3	57.8
199. Acrylonitrile [107-13-1]	C3H3N	199	77.4	0.0	90.9	0.3	87.3	1.41	108.7	22.2

Table 4. (Continued)

Training (Target & Results)			Experimental Data		ANN Predictions: Combined Model		ANN Predictions: Single output		PLS Predictions: Single Output	
No. Compound [CAS No]	Formula	Comp No.	Tb	Tf	Tb	Tf	Tb	Tf	Tb	Tf
202. Cyclopropanecarbonitrile [5500-21-0]	C4H5N	202	135.0	32.8	137.2	26.8	137.6	26.59	138.1	30.0
205. Hexanenitrile [628-73-9]	C6H11N	205	163.6	43.0	167.1	44.5	168.0	43.58	158.0	35.4
208. Allylamine [107-11-9]	C3H7N	208	56.5	-29.0	55.8	-20.9	52.9	-16.06	81.6	12.4
211. Butylamine [109-73-9]	C4H11N	211	77.9	-1.0	81.9	-6.0	81.9	-1.95	98.0	16.8
214. Diethylamine [109-89-7]	C4H11N	214	56.3	-23.0	84.1	4.4	81.9	-1.95	104.7	35.9
217. Pentylamine [110-58-7]	C5H13N	217	104.0	4.4	107.3	8.7	108.8	12.18	114.4	21.2
220. Hexylamine [111-26-2]	C6H15N	220	132.8	8.9	131.9	23.3	133.9	26.27	130.9	25.6
223. 1,3-Dimethylbutylamine [108-09-8]	C6H15N	223	107.5	12.8	117.8	14.9	119.7	18.16	121.4	23.1
226. Heptylamine [111-68-2]	C7H17N	226	155.0	35.0	155.6	37.6	157.3	40.26	147.3	30.0
229. Octylamine [111-86-4]	C8H19N	229	176.0	62.8	178.3	51.7	179.3	54.11	163.7	34.4
232. N,N-Diethylaniline [91-66-7]	C10H15N	232	217.1	85.0	222.0	84.8	213.4	74.46	208.2	69.8
235. p-t-Pentylaniline [2049-92-5]	C11H17N	235	260.0	101.7	248.0	97.6	252.9	101.47	236.4	78.3
238. Pyridine [110-86-1]	C5H5N	238	115.5	20.0	122.5	21.0	109.6	13.73	132.3	34.6
241. Quinoline [91-22-5]	C9H7N	241	237.1	92.0	229.9	91.2	239.5	90.26	220.3	74.4
244. Acetoanilide [103-84-4]	C8H9NO	244	304.0	173.0	304.0	173.0	303.9	172.33	304.1	173.1
247. N-Butylacetanilide [91-49-6]	C12H17NO	247	279.0	141.1	279.0	141.1	269.3	140.97	278.1	138.8
250. 2-Nitropropane [79-46-9]	C3H7NO2	250	120.1	24.0	102.2	11.9	100.0	15.67	114.5	30.4
253. m-Nitrotoluene [99-08-1]	C7H7NO2	253	232.6	106.0	226.4	101.1	228.9	96.36	217.0	82.3
256. Methyl isocyanate [624-83-9]	C2H3NO	256	38.0	-18.0	41.2	-22.0	39.9	-20.09	62.1	3.7
259. Cyclohexyl isocyanate [3173-53-3]	C7H11NO	259	169.0	48.9	165.1	51.7	167.3	50.83	144.8	25.9
262. 1-Butanethiol [109-79-5]	C4H10S	262	98.5	1.7	100.6	0.5	100.5	1.83	117.3	21.5
265. 1-Hexanethiol [111-31-9]	C6H14S	265	152.7	20.6	151.0	30.0	152.3	30.20	150.2	30.3
268. 1-Octanethiol [111-88-6]	C8H18S	268	199.0	68.0	197.8	58.7	197.4	58.17	183.1	39.1
271. Thiophene [110-02-1]	C4H4S	271	84.0	-1.1	99.2	12.5	98.0	14.19	109.2	24.8
274. Diallyl sulfide [592-88-1]	C6H10S	274	138.0	46.1	144.9	39.4	145.1	40.00	139.3	32.9
277. Dipropyl sulfone [598-03-8]	C6H14O2S	277	270.0	126.0	269.4	125.1	270.1	125.85	270.4	125.9
280. Allyl isothiocyanate [57-06-7]	C4H5NS	280	152.1	46.1	152.5	46.7	152.1	46.36	152.1	44.9
283. Ethyl chloride [75-00-3]	C2H5Cl	283	12.3	-43.0	14.2	-33.7	10.3	-30.85	54.0	19.2
286. Isopropyl chloride [75-29-6]	C3H7Cl	286	34.8	-32.0	31.3	-24.1	30.4	-21.99	64.5	22.0
289. 1-Bromobutane [109-65-9]	C4H9Br	289	101.6	23.9	103.2	21.2	100.5	20.69	112.6	38.0
292. 2-Fluoro-2-methylpropane [353-61-7]	C4H9F	292	12.1	-12.2	6.0	-46.4	8.7	-46.86	42.1	10.7
295. 1-Bromopentane [110-53-2]	C5H11Br	295	129.6	31.0	128.5	35.9	127.3	34.82	129.1	42.4
298. Fluorobenzene [462-06-6]	C6H5F	298	84.7	-45.0	92.3	9.1	101.2	12.84	122.9	56.7
301. 1-Bromohexane [111-25-1]	C6H13Br	301	156.0	57.2	153.0	50.3	152.2	48.88	145.5	46.8
304. o-Bromotoluene [95-46-5]	C7H7Br	304	181.8	78.9	185.8	72.6	189.0	77.84	193.4	84.0
307. m-Chlorotoluene [108-41-8]	C7H7Cl	307	161.7	50.6	152.1	49.4	151.6	53.83	167.1	73.9
310. 2-Iodotoluene [615-37-2]	C7H7I	310	211.0	90.0	204.8	82.6	205.0	82.87	205.3	85.3
313. 1-Iodoheptane [4282-40-0]	C7H15I	313	204.0	78.9	209.9	85.8	210.0	85.91	208.9	86.2
316. 1-Chlorooctane [111-85-3]	C8H17Cl	316	181.5	70.0	163.4	53.7	167.6	52.78	152.6	45.6
319. Acetyl chloride [75-36-5]	C2H3ClO	319	50.9	4.0	66.8	3.7	68.6	3.61	88.1	29.2
322. N,N-Dimethylhydrazine [57-14-7]	C2H8N2	322	63.0	-15.0	60.1	-12.8	42.3	-21.48	71.9	-0.5
325. 2-Chloropropionic acid [598-78-7]	C3H5ClO2	325	185.2	107.2	175.9	85.3	180.1	85.86	183.4	95.9
328. Propyl nitrate [627-13-4]	C3H7NO3	328	110.6	20.0	135.4	37.5	134.7	38.19	132.1	36.2
331. 2-(Methylamino)ethanol [109-83-1]	C3H9NO	331	169.5	73.9	150.0	64.0	150.1	58.07	154.5	69.4
334. Ethyl bromoacetate [105-36-2]	C4H7BrO2	334	158.8	47.8	156.5	63.1	158.4	60.54	154.9	53.5
337. Acetone cyanohydrin [75-86-5]	C4H7NO	337	209.0	74.0	190.3	79.0	192.6	79.69	179.8	61.3
340. 1,4-Thioxane [15980-15-1]	C4H8OS	340	148.9	42.2	126.7	35.3	127.9	33.01	122.7	29.5
343. 1,2-Dimethoxyethane [110-71-4]	C4H10O2	343	84.7	-1.7	77.0	3.4	80.9	-3.41	89.9	26.1
346. Diethylene glycol [111-46-6]	C4H10O3	346	245.0	124.0	229.3	126.6	234.4	124.90	208.9	97.2
349. 2-(2-Aminoethylamino)ethanol[111-41-1]	C4H12N2O	349	238.9	129.0	233.6	115.0	237.2	110.54	206.0	73.8
352. 2,4-Pentanedione [123-54-6]	C5H8O2	352	140.5	34.0	154.2	48.2	161.1	43.73	150.0	41.9
355. 3-Ethoxypropionic acid [4324-38-3]	C5H10O3	355	218.9	107.2	213.7	100.2	213.3	99.50	210.0	99.3
358. Bromopentafluorobenzene [344-04-7]	C6BrF5	358	137.0	87.0	139.4	82.7	138.4	82.98	129.5	63.9
361. 2,4-Dichlorophenol [120-83-2]	C6H4Cl2O	361	209.5	113.9	233.6	125.5	226.8	117.23	216.4	112.2
364. Ethyl acetoacetate [141-97-9]	C6H10O3	364	180.4	57.2	179.6	84.2	178.9	62.67	173.3	51.5
366. Adipic acid [124-04-9]	C6H10O4	366	354.8	196.0	348.6	202.1	349.1	200.88	330.0	172.4
367. Ethylene glycol diacetate [111-55-7]	C6H10O4	367	190.5	88.3	182.7	63.6	190.8	63.99	177.7	55.9
370. 2-Ethoxyethyl acetate [111-15-9]	C6H12O3	370	156.0	47.2	149.3	43.7	143.7	45.16	150.3	45.4
373. 1,2-Diethoxyethane [629-14-4]	C6H14O2	373	124.0	35.0	122.2	26.2	122.3	24.52	122.8	34.9
376. 2-Chlorobenzotrifluororide [88-16-4	C7H4ClF3	376	152.2	59.0	147.7	68.3	145.3	66.69	141.9	65.4
379. Salicylaldehyde [90-02-8]	C7H6O2	379	195.0	77.8	226.0	101.3	216.5	95.15	202.7	76.8
382. Phenacyl chloride [532-27-4]	C8H7ClO	382	244.5	118.0	242.2	105.9	232.5	105.43	225.4	90.4
385. 2-Phenoxyethanol [122-99-6]	C8H10O2	385	244.7	121.1	248.6	126.3	238.6	122.42	244.0	110.9
388. Bis[2-(2-chloroethoxy)ethyl] ether [638-556-2]	C8H16Cl2O3	388	251.0	121.1	247.9	122.1	252.5	135.01	217.1	70.8
391. Dibutoxymethane [2568-90-3]	C9H20O2	391	177.0	60.0	183.7	59.2	177.3	65.29	172.1	48.1
394. Pentyl salicylate [2050-08-0]	C12H16O	394	266.7	132.0	282.2	135.3	279.4	159.82	314.5	133.1
397. Anthraquinone [84-65-1]	C14H8O2	397	379.8	185.0	383.7	185.6	379.1	186.99	373.2	150.5
400. Ethyl(o-(ethoxycarbonyl)-benzoyloxyacetate) [84-72-0]	C14H16O6	400	453.0	188.0	447.3	187.1	451.6	178.94	388.9	141.0

these pairs of **n** and σ should help pinpoint the value of **n** and σ required to achieve minimum validation error, i.e. the optimized network configuration. The versatile nonlinear interpolation power of splines was used to generated the response surface and to pick the optimum network configuration for the data. The ranges of σ and **n** examined were 1−20 and 5−60, respectively, represented by [26-**(5-60)**$_{[1-20]}$-2] for 26 input and two output neurons. Each range was divided into seven resulting a total of 49 equally spaced initial modeling points indicated by the small circles in Figure 2a,b. The *validation error* outputs of 49 networks were used to estimated the error profiles over a 50 × 50 grid. Thus from the 49 network models, an error interpolation for the rest of the 2451 models were estimated by means of biharmonic splines, and the response surface output is shown in Figure 2a,b. The use of validation error instead of the training error for optimization eliminates the chances of overtraining the network. After obtaining the optimized network, a further robustness analysis was performed combining the validation and test data sets, randoming their positions, splitting the randomized data into two, and using the each half to test the optimized model. This robustness analysis is called random split cross-validation in this paper, 10 outputs of this analysis were studied for the optimized model, and the results are discussed in the next section. Single output models for T_b and T_f, for the configuration [26-**(5-60)**$_{[1-20]}$-1], were also studied.

Model generation for PLS used the same data sets as in the RBF neural models. The strategy used was to evaluate the prediction performance of PLS models as a function of the number of factors. Since 26 is the maximum number of factors, the factor range was from 1 to 26. The best model was selected as the model with the lowest validation error. The test data set was then used to check the true prediction ability of the optimum PLS model. Figure 7a,b shows the error profile for training and validation. Both double and single output models were studied.

Table 5. (a) Input Parameters for Validation Data Set and (b) Output Results for Validation Data Sets

Validation (Inputs)		Descriptors																												
No. Compound [CAS No]	Comp No.	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO
2. Cyclopentane [287-92-3]	2	2.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5. 4-Methyl-1,3-pentadiene [926-56-7]	5	2.77	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8. 2,2-Dimethylbutane [75-83-2]	8	2.561	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11. Heptane [142-82-5]	11	3.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14. 2,4,4-Trimethyl-1-pentene [107-39-1]	14	3.061	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17. Octane [111-65-9]	17	3.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20. 3-Ethyl-4-methylhexane [3074-77-9]	20	4.256	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23. Decane [124-18-5]	23	4.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26. Tridecane [629-50-5]	26	6.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29. Pentadecane [629-62-9]	29	7.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32. Octadecane [593-45-3]	32	8.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35. Toluene [108-88-3]	**35**	**3.394**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
38. m-Xylene [108-38-3]	38	3.788	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41. *ƒ¿*-Methylstyrene [98-83-9]	41	4.305	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44. 1,2,4-Trimethylbenzene [95-63-6]	44	4.198	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47. Butylbenzene [104-51-8]	47	4.932	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50. p-Diethylbenzene [105-05-5]	50	4.864	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53. Pentylbenzene [538-68-1]	53	5.432	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56. 1-Phenylheptane [1078-71-3]	56	6.432	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59. 2-Isopropylbiphenyl [19486-60-3]	59	7.288	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62. Allyl alcohol [107-18-6]	62	1.914	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65. trans-2-Buten-1-ol [504-61-0]	65	2.414	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68. 1-Butanol [71-36-3]	68	2.414	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71. t-Butyl alcohol [75-65-0]	71	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
74. 1-Pentanol [71-41-0]	74	2.914	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
77. Cyclohexanol [108-93-0]	77	3.394	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
80. Benzyl alcohol [100-51-6]	80	3.932	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
83. 2-Phenylethanol [60-12-8]	83	4.432	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86. 2-Ethyl-1-hexanol [104-76-7]	86	4.346	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
89. 2-Butyl-1-octanol [3913-02-8]	89	6.346	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
92. m-Cresol [108-39-4]	92	3.788	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95. 2-Naphthol [135-19-3]	95	5.36	10	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98. 2-Phenylphenol [90-43-7]	98	6.377	12	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
101. Ethyl methyl ether [540-67-0]	101	1.914	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
104. Tetrahydrofuran [109-99-9]	104	2.5	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107. 3,4-Dihydro-2H-pyran [110-87-2]	107	3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
110. 2-Methyltetrahydrofuran [96-47-9]	110	2.894	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113. Butyl ethyl ether [628-81-9]	113	3.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
116. Dibutyl ether [142-96-1]	116	4.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
119. Dihexyl ether [112-58-3]	119	6.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
122. Bis(2-ethyl hexyl)ether [10143-60-9]	122	8.278	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
125. Propionaldehyde [123-38-6]	125	1.914	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
128. Butyraldehyde [123-72-8]	128	2.414	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
131. 1-Octanal [124-13-0]	131	4.414	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
134. Methyl vinyl ketone [78-94-4]	134	2.27	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
137. 2-Pentanone [107-87-9]	137	2.77	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
140. 4-Methyl-3-penten-2-one [141-79-7]	140	3.126	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
143. 2-Heptanone [110-43-0]	143	3.77	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
146. Acetophenone [98-86-2]	146	4.305	6	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
149. 2,6-Dimethyl-4-heptanone [108-83-8]	149	4.52	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
152. Propionic acid [79-09-4]	152	2.27	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
155. Pentanoic acid [109-52-4]	155	3.27	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
158. Benzoic acid [65-85-0]	158	4.304	6	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
160. Octanoic acid [124-07-2]	**161**	**1.914**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
164. Vinyl acetate [108-05-4]	164	2.77	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
167. Propyl formate [110-74-7]	167	2.914	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
170. Isopropenyl acetate [108-22-5]	170	3.126	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
173. Ethyl propionate [105-37-3]	173	3.308	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
176. Propyl acetate [109-60-4]	176	3.27	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
179. Pentyl formate [638-49-3]	179	3.914	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
182. Pentyl acetate [628-63-7]	182	4.27	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
185. Butyl propionate [590-01-2]	185	4.308	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
188. Cyclohexyl acetate [622-45-7]	188	4.787	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
191. Ethyl benzoate [93-89-0]	191	5.343	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
194. Butyl isovalerate [109-19-3]	194	5.164	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
197. p-t-Pentylphenyl acetate	197	7.305	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
200. Propionitrile [107-12-0]	200	1.914	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
203. Butyronitrile [109-74-0]	203	2.414	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
206. Benzonitrile [100-47-0]	206	3.932	6	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
209. Isopropylamine [75-31-0]	209	1.732	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
212. s-Butylamine [33966-50-6]	212	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
215. Piperidine [110-89-4]	215	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
218. 2-Pentanesmine [63493-28-7]	218	2.77	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
221. Dipropylamine [142-84-7]	221	3.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
224. o-Toluidine [95-53-4]	224	3.804	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
227. 2,3-Dimethylaniline [87-59-2]	227	4.215	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
230. Dibutylamine [111-92-2]	230	4.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
233. Decylamine [2016-57-1]	233	5.414	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
236. Diphenylamine [122-39-4]	236	6.449	12	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
239. 2-Methylpyridine [109-06-8]	239	3.394	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
242. N-Ethylacetamide [625-50-3]	242	2.77	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
245. p-Acetotoluide [103-89-9]	245	5.182	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
248. Nitroethane [79-24-3]	248	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
251. Nitrobenzene [98-95-3]	251	4.304	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
254. 1-Nitronaphthalene [86-57-7]	254	6.288	10	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
257. Butyl isocyanate [111-36-4]	257	3.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
260. Ethanethiol [75-08-1]	260	1.414	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
263. 1-Pentanethiol [110-66-7]	263	2.914	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
266. Phenylmethanethiol [100-53-8]	266	3.932	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
269. 1-Dodecanethiol [112-55-0]	269	6.414	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
272. Diethyl sulfide [352-93-2]	272	2.414	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
275. Dibutyl sulfide [544-40-1]	275	4.414	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
278. Dibutyl sulfone [598-04-9]	278	5.121	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
281. Butyl isothiocyanate [592-82-5]	281	3.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
284. Allyl chloride [107-05-1]	284	1.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
287. Chloroprene [126-99-8]	287	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
290. 2-Chlorobutane [78-86-4]	290	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
293. 1-Iodobutane [542-69-8]	293	2.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
296. Bromobenzene [108-86-1]	296	3.394	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0

Table 5. (Continued)

Validation (Inputs) — Descriptors

No. Compound [CAS No]	Comp No.	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO
299. Iodobenzene [591-50-4]	299	3.394	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
302. 1-Chlorohexane [544-10-5]	302	3.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
305. p-Bromotoluene [106-38-7]	305	3.788	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
308. Benzyl chloride [100-44-7]	308	3.932	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
311. 3-Iodotoluene [625-95-6]	311	3.788	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
314. 1-Chloro-4-ethylbenzene [622-98-0]	314	4.326	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
317. 4-Bromobiphenyl [92-66-0]	317	6.36	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
320. 2-Chloroethanol [107-07-3]	320	1.914	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
323. 2-Chloro-1-propanol [78-89-7]	323	2.27	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
326. Ethyl chloroformate [541-41-3]	326	2.77	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
329. 2-Methoxyethanol [109-86-4]	329	2.414	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
332. Succinonitrile [110-61-2]	332	2.914	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
335. 2-Chloroethyl acetate [542-58-5]	335	3.27	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
338. 2,2'-Dichlorodiethyl ether [111-44-2]	338	3.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
341. 3-(Methylthio)propionaldehyde[3268-49-3]	341	2.914	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
344. 2-Ethoxyethanol [110-80-5]	344	2.914	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
347. 3-Methoxypropylamine [5332-73-0]	347	2.914	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
350. Diethylenetriamine [111-40-0]	350	3.414	0	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0
353. 3-Ethoxypropionaldehyde [2806-85-1]	353	3.414	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
356. 2-Methoxyethyl acetate [110-49-6]	356	3.77	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
359. 1-Chloro-2,4-dinitrobenzene [97-00-7]	359	6.112	6	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	0
362. o-Dinitrobenzene [528-29-0]	362	5.826	6	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
365. Ethyl acetylglycolate [623-86-9]	365	4.664	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
368. 3-Isopropoxypropionitrile [110-47-4]	368	4.27	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
371. 2-Butoxyethanol [111-76-2]	371	3.914	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
374. 2-(2-Ethoxyethoxy)ethanol [111-90-0	374	4.414	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
377. 4-Chlorophenyl isocyanate [104-12-1	377	4.626	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1
380. Furfuryl acetate [623-17-6]	380	4.788	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
383. Methyl salicylate [119-36-8]	383	5.253	6	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
386. p-Phenetidine [156-43-4]	386	4.826	6	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
389. 2-Butoxyethyl acetate [112-07-2]	389	5.27	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
392. Dimethyl phthalate [131-11-3]	392	6.702	6	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
395. 2-Chloro-4-t-pentylphenyl methyl ether	395	6.421	6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
398. 2-Biphenylyl 2-chloroethyl ether	398	7.915	12	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0

Validation (Target & Results)

No. Compound [CAS No]	Formula	Comp No.	Experimental Data Tb	Experimental Data Tf	ANN Predictions Combined Model Tb	ANN Predictions Combined Model Tf	ANN Predictions Single output Tb	ANN Predictions Single output Tf	PLS Predictions Single Output Tb	PLS Predictions Single Output Tf
2. Cyclopentane [287-92-3]	C5H10	2	49.3	-37.0	52.1	-25.6	50.7	-24.00	82.2	22.0
5. 4-Methyl-1,3-pentadiene [926-56-7]	C6H10	5	75.6	-34.0	65.8	-17.7	65.3	-16.36	91.0	24.4
8. 2,2-Dimethylbutane [75-83-2]	C6H14	8	49.7	-48.0	55.2	-23.8	54.1	-22.28	84.2	22.5
11. Heptane [142-82-5]	C7H16	11	98.4	-1.0	97.7	1.2	98.0	1.80	112.2	30.0
14. 2,4,4-Trimethyl-1-pentene [107-39-1]	C8H16	14	101.1	-5.0	80.4	-9.1	80.5	-8.18	100.6	26.9
17. Octane [111-65-9]	C8H18	17	125.7	15.0	121.6	15.6	121.5	15.85	128.6	34.4
20. 3-Ethyl-4-methylhexane [3074-77-9]	C9H20	20	140.0	24.0	137.4	25.4	136.8	25.39	139.9	37.4
23. Decane [124-18-5]	C10H22	23	174.1	46.0	166.6	44.0	164.6	43.52	161.5	43.2
26. Tridecane [629-50-5]	C13H28	26	235.4	79.0	227.5	85.3	223.5	83.17	210.6	56.4
29. Pentadecane [629-62-9]	C15H32	29	270.6	132.0	263.5	111.9	262.3	107.74	243.7	65.2
32. Octadecane [593-45-3]	C18H38	32	316.7	165.0	310.7	150.7	325.3	140.87	293.0	78.4
35. Toluene [108-88-3]	**C7H8**	**35**	**110.6**	**4.0**	114.6	15.7	116.9	21.82	146.6	63.6
38. m-Xylene [108-38-3]	C8H10	38	139.1	27.0	134.8	27.5	139.6	32.65	159.5	67.1
41. *p*-Methylstyrene [98-83-9]	C9H10	41	163.5	53.9	160.4	42.6	165.0	46.69	176.5	71.6
44. 1,2,4-Trimethylbenzene [95-63-6]	C9H12	44	169.2	44.0	155.2	39.5	159.9	43.80	173.0	70.7
47. Butylbenzene [104-51-8]	C10H14	47	183.3	59.0	190.0	60.6	193.8	63.35	197.1	77.2
50. p-Diethylbenzene [105-05-5]	C10H14	50	183.8	57.0	186.8	58.7	190.8	61.56	194.9	76.6
53. Pentylbenzene [538-68-1]	C11H16	53	202.2	65.0	212.3	74.6	215.4	76.29	213.5	81.6
56. 1-Phenylheptane [1078-71-3]	C13H20	56	233.0	95.0	253.9	101.8	256.5	101.03	246.4	90.4
59. 2-Isopropylbiphenyl [19486-60-3]	C15H16	59	270.0	140.6	296.6	135.1	326.6	145.02	309.6	131.7
62. Allyl alcohol [107-18-6]	C3H6O	62	96.9	21.0	87.3	18.4	85.5	19.55	112.7	50.3
65. trans-2-Buten-1-ol [504-61-0]	C4H8O	65	121.2	32.8	113.6	31.5	114.3	33.68	129.2	54.7
68. 1-Butanol [71-36-3]	C4H10O	68	117.7	29.0	113.6	31.5	114.3	33.68	129.2	54.7
71. t-Butyl alcohol [75-65-0]	C4H10O	71	82.5	11.0	91.9	19.0	90.6	21.98	115.5	51.1
74. 1-Pentanol [71-41-0]	C5H12O	74	137.8	33.0	139.1	48.3	140.9	47.77	145.6	59.1
77. Cyclohexanol [108-93-0]	C6H12O	77	161.1	68.0	162.7	60.3	164.8	61.22	161.4	63.3
80. Benzyl alcohol [100-51-6]	C7H8O	80	205.4	93.0	202.0	86.0	197.2	91.24	214.1	101.8
83. 2-Phenylethanol [60-12-8]	C8H10O	83	218.9	102.0	226.2	100.5	220.9	104.52	230.5	106.2
86. 2-Ethyl-1-hexanol [104-76-7]	C8H18O	86	183.5	73.0	207.1	87.4	207.3	87.48	192.7	71.7
89. 2-Butyl-1-octanol [3913-02-8]	C12H26O	89	252.2	110.0	268.9	141.5	264.6	139.37	258.4	89.3
92. m-Cresol [108-39-4]	C7H8O	92	202.7	86.0	188.7	75.2	184.1	85.32	187.8	95.0
95. 2-Naphthol [135-19-3]	C10H8O	95	296.0	153.0	243.1	114.5	280.7	128.80	262.8	131.4
98. 2-Phenylphenol [90-43-7]	C12H10O	98	287.0	123.8	267.6	132.3	325.7	159.18	307.9	151.6
101. Ethyl methyl ether [540-67-0]	C3H8O	101	6.6	-37.2	26.4	-31.7	24.7	-35.70	60.0	17.1
104. Tetrahydrofuran [109-99-9]	C4H8O	104	66.0	-14.0	55.1	-16.0	55.9	-19.21	79.2	22.2
107. 3,4-Dihydro-2H-pyran [110-87-2]	C5H8O	107	86.0	-18.0	79.6	-2.8	80.6	-5.10	95.7	26.6
110. 2-Methyltetrahydrofuran [96-47-9]	C5H10O	110	80.0	-11.1	74.5	-5.6	75.5	-8.09	92.2	25.7
113. Butyl ethyl ether [628-81-9]	C6H14O	113	92.3	4.4	99.4	8.0	99.7	6.56	109.3	30.3
116. Dibutyl ether [142-96-1]	C8H18O	116	142.0	25.0	144.6	33.6	142.2	34.47	142.1	39.1
119. Dihexyl ether [112-58-3]	C12H26O	119	226.2	77.0	224.7	83.0	217.9	87.69	207.9	56.7
122. Bis(2-ethyl hexyl)ether [10143-60-9]	C16H34O	122	269.4	112.8	286.4	127.1	290.7	131.71	269.2	73.1
125. Propionaldehyde [123-38-6]	C3H6O	125	47.9	-30.0	44.9	-25.2	51.4	-24.08	59.8	-6.3
128. Butyraldehyde [123-72-8]	C4H8O	128	74.8	-6.7	71.0	-10.3	79.7	-10.03	76.0	-1.9
131. 1-Octanal [124-13-0]	C8H16O	131	168.0	52.0	167.4	47.4	174.4	45.84	141.8	15.7
134. Methyl vinyl ketone [78-94-4]	C4H6O	134	81.4	-7.0	75.8	-4.6	76.3	-4.90	98.2	27.2
137. 2-Pentanone [107-87-9]	C5H10O	137	101.9	7.2	101.6	10.1	103.8	9.15	114.6	31.6
140. 4-Methyl-3-penten-2-one [141-79-7]	C6H10O	140	129.8	31.0	119.5	20.5	122.2	19.15	126.3	34.7
143. 2-Heptanone [110-43-0]	C7H14O	143	150.4	47.0	150.7	39.1	153.2	37.14	147.5	40.4
146. Acetophenone [98-86-2]	C8H8O	146	202.0	77.0	199.9	69.1	196.4	70.46	200.1	78.9
149. 2,6-Dimethyl-4-heptanone [108-83-8]	C9H18O	149	168.2	49.0	185.1	60.3	186.3	57.80	172.2	47.0
152. Propionic acid [79-09-4]	C3H6O2	152	140.8	51.0	137.2	49.8	135.0	51.80	163.6	85.8
155. Pentanoic acid [109-52-4]	C5H10O2	155	185.5	86.0	188.6	80.0	188.9	80.72	196.5	94.8
158. Benzoic acid [65-85-0]	C7H6O2	158	250.0	121.0	249.8	118.6	254.6	122.79	265.4	137.5
160. Octanoic acid [124-07-2]	**C8H16O2**	**161**	**32.0**	**-10.0**	27.5	-24.0	35.4	-25.73	75.7	24.4
164. Vinyl acetate [108-05-4]	C4H6O2	164	73.1	-8.0	73.5	-0.4	79.4	-1.58	103.9	32.0
167. Propyl formate [110-74-7]	C4H8O2	167	81.5	-3.0	81.1	3.5	86.2	2.48	108.6	33.2
170. Isopropenyl acetate [108-22-5]	C5H8O2	170	97.2	15.6	92.1	9.2	96.1	8.47	115.6	35.1
173. Ethyl propionate [105-37-3]	C5H10O2	173	99.1	12.0	101.4	14.1	104.3	13.60	121.6	36.7
176. Propyl acetate [109-60-4]	C5H10O2	176	101.6	12.0	99.4	13.1	102.6	12.53	120.3	36.4

Table 5. (Continued)

Validation (Target & Results)					ANN Predictions				PLS Predictions	
			Experimental Data		Combined Model		Single output		Single Output	
No. Compound [CAS No]	Formula	Comp No.	Tb	Tf	Tb	Tf	Tb	Tf	Tb	Tf
179. Pentyl formate [638-49-3]	C6H12O2	179	132.0	26.7	131.7	30.2	130.3	30.60	141.5	42.0
182. Pentyl acetate [628-63-7]	C7H14O2	182	149.2	23.9	149.0	39.6	144.7	40.49	153.2	45.2
185. Butyl propionate [590-01-2]	C7H14O2	185	146.8	32.0	150.8	40.6	146.2	41.55	154.4	45.5
188. Cyclohexyl acetate [622-45-7]	C8H14O2	188	176.7	58.0	173.3	53.0	164.7	54.71	170.2	49.7
191. Ethyl benzoate [93-89-0]	C9H10O2	191	212.9	88.0	220.6	83.3	209.0	80.50	223.5	88.4
194. Butyl isovalerate [109-19-3]	C9H18O2	194	150.0	53.0	190.4	62.6	178.8	64.92	182.6	53.0
197. p-t-Pentylphenyl acetate	C13H18O2	197	265.0	115.6	304.5	130.6	283.6	127.46	287.9	105.7
200. Propionitrile [107-12-0]	C3H5N	200	97.4	2.0	90.9	0.3	87.3	1.41	108.7	22.2
203. Butyronitrile [109-74-0]	C4H7N	203	117.9	16.7	117.1	15.2	116.2	15.49	125.1	28.6
206. Benzonitrile [100-47-0]	C7H5N	206	191.1	71.7	205.0	71.1	210.5	74.60	210.0	73.7
209. Isopropylamine [75-31-0]	C3H9N	209	32.4	-17.0	46.1	-26.3	41.8	-21.19	75.6	10.8
212. s-Butylamine [33966-50-6]	C4H11N	212	63.5	-9.0	74.5	-10.3	73.7	-6.02	93.3	15.6
215. Piperidine [110-89-4]	C5H11N	215	105.6	16.0	113.8	21.6	113.3	14.61	123.9	41.1
218. 2-Pentaneamine [63493-28-7]	C5H13N	218	92.0	-6.7	100.1	4.5	101.3	8.11	109.7	20.0
221. Dipropylamine [142-84-7]	C6H15N	221	109.2	17.0	134.0	33.6	133.9	26.27	137.5	44.7
224. o-Toluidine [95-53-4]	C7H9N	224	199.7	85.0	186.6	48.0	173.0	55.37	178.7	62.8
227. 2,3-Dimethylaniline [87-59-2]	C8H11N	227	221.5	97.0	186.8	59.9	193.3	66.49	192.2	66.5
230. Dibutylamine [111-92-2]	C8H19N	230	159.6	40.0	180.4	62.0	179.3	54.11	170.4	53.5
233. Decylamine [2016-57-1]	C10H23N	233	217.0	99.0	221.1	79.4	220.0	81.13	196.6	43.2
236. Diphenylamine [122-39-4]	C12H11N	236	302.0	152.8	291.3	138.0	322.0	146.43	307.3	138.9
239. 2-Methylpyridine [109-06-8]	C6H7N	239	128.5	26.0	143.2	32.9	131.5	24.79	145.2	38.1
242. N-Ethylacetamide [625-50-3]	C4H9NO	242	205.0	110.0	175.0	87.7	170.9	85.99	202.8	121.6
245. p-Acetotoluide [103-89-9]	C9H11NO	245	307.0	168.0	321.9	184.1	321.3	182.58	317.1	176.6
248. Nitroethane [79-24-3]	C2H5NO2	248	115.0	28.0	82.8	0.5	79.2	5.03	102.2	27.1
251. Nitrobenzene [98-95-3]	C6H5NO2	251	211.0	87.8	207.6	89.6	210.6	85.85	204.1	78.8
254. 1-Nitronaphthalene [86-57-7]	C10H7NO2	254	304.0	164.0	303.5	159.0	322.6	154.47	292.6	118.8
257. Butyl isocyanate [111-36-4]	C5H9NO	257	115.0	26.7	117.5	22.4	121.0	22.38	111.4	16.9
260. Ethanethiol [75-08-1]	C2H6S	260	35.0	-17.0	47.0	-29.8	40.5	-26.50	84.5	12.7
263. 1-Pentanethiol [110-66-7]	C5H12S	263	126.6	16.3	126.2	15.3	127.4	16.03	133.8	25.9
266. Phenylmethanethiol [100-53-8]	C7H8S	266	195.0	70.0	190.6	58.0	196.1	62.51	202.2	68.7
269. 1-Dodecanethiol [112-55-0]	C12H26S	269	275.0	87.8	280.0	113.6	275.5	111.15	248.8	56.7
272. Diethyl sulfide [352-93-2]	C4H10S	272	92.1	-9.4	94.8	10.0	93.2	11.75	106.4	24.1
275. Dibutyl sulfide [544-40-1]	C8H18S	275	188.9	76.7	191.5	67.9	190.4	67.81	172.1	41.7
278. Dibutyl sulfone [598-04-9]	C8H18O2S	278	291.0	143.0	313.3	153.0	311.9	153.04	303.2	134.7
281. Butyl isothiocyanate [592-82-5]	C5H9NS	281	168.0	65.6	177.1	61.2	177.1	60.40	168.5	49.3
284. Allyl chloride [107-05-1]	C3H5Cl	284	45.1	-32.0	41.0	-18.7	41.4	-16.91	70.5	23.6
287. Chloroprene [126-99-8]	C4H5Cl	287	59.4	-20.0	59.6	-8.1	62.2	-6.93	82.2	26.8
290. 2-Chlorobutane [78-86-4]	C4H9Cl	290	68.3	-15.0	59.6	-8.1	62.2	-6.93	82.2	26.8
293. 1-Iodobutane [542-69-8]	C4H9I	293	129.5	33.0	135.7	41.7	134.2	43.41	159.6	73.0
296. Bromobenzene [108-86-1]	C6H5Br	296	156.2	51.0	164.9	60.5	167.6	66.61	179.9	80.4
299. Iodobenzene [591-50-4]	C6H5I	299	188.3	74.0	195.1	79.6	199.7	85.89	226.8	115.4
302. 1-Chlorohexane [544-10-5]	C6H13Cl	302	132.2	35.0	116.9	25.3	122.2	25.13	119.8	36.8
305. p-Bromotoluene [106-38-7]	C7H7Br	305	184.5	85.0	185.0	72.1	188.1	77.38	192.8	83.9
308. Benzyl chloride [100-44-7]	C7H7Cl	308	179.3	67.0	159.3	53.6	158.9	57.72	171.8	75.2
311. 3-Iodotoluene [625-95-6]	C7H7I	311	191.6	82.2	204.0	82.2	204.3	82.39	204.8	85.1
314. 1-Chloro-4-ethylbenzene [622-98-0]	C8H9Cl	314	184.4	64.0	178.6	64.9	177.9	68.26	184.8	78.6
317. 4-Bromobiphenyl [92-66-0]	C12H9Br	317	311.2	143.9	300.8	147.2	329.6	163.16	312.4	140.3
320. 2-Chloroethanol [107-07-3]	C2H5ClO	320	128.7	60.0	106.6	40.6	109.7	42.94	120.3	57.1
323. 2-Chloro-1-propanol [78-89-7]	C3H7ClO	323	133.5	51.7	125.4	51.3	130.4	52.96	132.0	60.2
326. Ethyl chloroformate [541-41-3]	C3H5ClO2	326	92.5	16.0	92.8	23.8	103.6	21.80	111.4	38.8
329. 2-Methoxyethanol [109-86-4]	C3H8O2	329	124.5	39.0	116.6	41.2	119.4	38.31	126.2	55.0
332. Succinonitrile [110-61-2]	C4H4N2	332	266.0	132.2	210.5	73.1	213.5	70.41	187.3	36.3
335. 2-Chloroethyl acetate [542-58-5]	C4H7ClO2	335	143.9	66.1	118.6	37.2	126.8	35.80	127.9	43.2
338. 2,2'-Dichlorodiethyl ether [111-44-2]	C4H8Cl2O	338	178.6	55.0	136.5	58.0	148.6	52.14	124.4	43.9
341. 3-(Methylthio)propionaldehyde[3268-49-3]	C4H8OS	341	165.0	61.1	143.4	42.5	152.9	42.11	119.5	5.4
344. 2-Ethoxyethanol [110-80-5]	C4H10O2	344	135.1	43.3	141.3	54.4	144.1	52.39	142.7	59.4
347. 3-Methoxypropylamine [5332-73-0]	C4H11NO	347	116.1	32.2	109.6	17.0	112.3	16.89	111.5	21.5
350. Diethylenetriamine [111-40-0]	C4H13N3	350	204.0	98.0	200.5	77.3	205.9	74.16	174.8	35.9
353. 3-Ethoxypropionaldehyde [2806-85-1]	C5H10O2	353	135.0	38.0	122.5	25.7	132.0	22.78	106.0	7.2
356. 2-Methoxyethyl acetate [110-49-6]	C5H10O3	356	144.4	49.0	125.6	32.1	124.8	31.27	133.8	41.0
359. 1-Chloro-2,4-dinitrobenzene [97-00-7]	C6H3ClN2O4	359	315.0	194.0	348.5	207.4	344.3	189.42	298.7	108.7
362. o-Dinitrobenzene [528-29-0]	C6H4N2O4	362	319.0	150.0	312.7	173.8	314.0	157.82	275.1	97.6
365. Ethyl acetylglycolate [623-86-9]	C6H10O4	365	179.0	82.0	184.5	84.5	192.1	85.02	179.0	56.3
368. 3-Isopropoxypropionitrile [110-47-4]	C6H11NO	368	187.8	68.3	207.1	72.9	205.7	71.87	183.2	43.1
371. 2-Butoxyethanol [111-76-2]	C6H14O2	371	171.2	65.6	188.1	80.3	188.3	80.23	175.5	68.1
374. 2-(2-Ethoxyethoxy)ethanol [111-90-0	C6H14O3	374	195.0	94.0	208.5	96.2	206.8	97.26	189.0	72.8
377. 4-Chlorophenyl isocyanate [104-12-1	C7H4ClNO	377	204.0	110.0	219.7	98.3	221.5	99.99	200.3	69.9
380. Furfuryl acetate [623-17-6]	C7H8O3	380	183.0	85.0	172.8	55.5	162.3	59.36	167.3	50.0
383. Methyl salicylate [119-36-8]	C8H8O3	383	223.3	96.0	235.7	109.4	215.0	111.49	248.8	115.5
386. p-Phenetidine [156-43-4]	C8H11NO	386	249.9	116.1	215.1	89.6	217.6	87.71	209.3	72.1
389. 2-Butoxyethyl acetate [112-07-2]	C8H16O3	389	188.0	71.0	194.0	68.4	179.1	72.35	183.1	54.2
392. Dimethyl phthalate [131-11-3]	C10H10O4	392	282.4	146.0	301.8	125.9	283.4	118.91	281.0	108.0
395. 2-Chloro-4-t-pentylphenyl methyl ether	C12H17ClO	395	273.0	110.0	266.6	129.0	259.9	125.74	250.7	97.3
398. 2-Biphenylyl 2-chloroethyl ether	C14H13ClO	398	322.8	160.0	322.9	172.0	338.5	173.88	334.8	144.2

RESULTS AND DISCUSSION

In Figure 2a,b the response surface generated from the validation error output for the set of 49 equally spaced network configuration is described. The axes consist of the Gaussian spread parameter and the number of neurons in the hidden layer. The contour representation in Figure 2b shows the average absolute error of validation for the combined output for T_f and T_b. It suggests that the combination of spread and number of neurons required for an optimum RBF network operation is not a simple linear relationship. The figure shows a relatively wide region capable of low validation error can be found in the spread and neuron range 6−20 and 25−60, respectively. Within this boundary the two regions indicated by solid square in Figure 2b suggest regions of optimal network configuration. The best network configuration identified for testing the model is located at 36 neurons and a spread parameter of 16.5 for the double target [26-**36**$_{[16.5]}$-2] output network schematically depicted in Figure 1. The generated response surface in Figure 2a,b provides the freedom and flexibility to select a suitable network configuration capable of modeling the target properties. This flexibility enabled explicit selection of the minimum number of neurons required to predict both T_f and T_b with minimum error. Although models with more than 36 neurons such as [26-**55**$_{[7]}$-2] could be generated, stable models in neural networks generally have the minimum number of neurons possible in the hidden layer. This is similar to selection of the number of factors in PLS models.

Table 6. (a) Input Parameters for Testing Data Set and (b) Output Results for Testing Data Sets

Testing (Inputs)	Descriptors																												
No. Compound [CAS No]	Comp No.	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO
3. Pentane [109-66-0]	3	2.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6. Cyclohexane [110-82-7]	6	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9. 2,3-Dimethylbutane [79-29-8]	9	2.643	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12. 2,4-Dimethylpentane [108-08-7]	12	3.126	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15. trans-1,4-Dimethylcyclohexane [2207-04-7]	15	3.788	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18. 2,2,4-Trimethylpentane [540-84-1]	18	3.417	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21. Dipentene [138-86-3]	21	4.698	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24. Undecane [1120-21-4]	24	5.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27. 1-Tetradecene [1120-36-1]	27	6.524	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30. Hexadecane [544-76-3]	30	7.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33. Nonadecane [629-92-5]	33	9.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36. Styrene [100-42-5]	36	3.932	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39. Ethylbenzene [100-41-0]	39	3.932	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42. Cumene [98-82-8]	42	4.305	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45. Naphthalene [91-20-3]	45	4.966	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48. Isobutylbenzene [538-93-2]	48	4.788	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51. p-Cymen [99-87-6]	51	4.698	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54. Biphenyl [92-52-4]	54	5.966	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57. Anthracene [120-12-7]	57	6.933	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60. Methanol [67-56-1]	60	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63. 1-Propanol [71-23-8]	63	1.914	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66. 3-Buten-1-ol [627-27-0]	66	2.414	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69. 2-Butanol [78-92-2]	69	2.27	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72. Cyclopentanol [96-41-3]	72	2.893	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75. Isopentyl alcohol [123-51-3]	75	2.77	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
78. 1-Hexanol [11-27-3]	78	3.414	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
81. 4-Methyl-cyclohexanol [589-91-3]	81	3.787	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84. 1-Octanol [111-87-5]	84	4.414	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
87. 1-Nonanol [143-08-8]	87	4.914	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90. Phenol [108-95-2]	90	3.394	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93. p-Cresol [106-44-5]	93	3.788	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
96. o-t-Pentylphenol [3279-27-4]	**96**	**5.577**	**6**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
99. Nonylphenol [25154-52-3]	99	7.826	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
102. Ethyl vinyl ether [109-92-2]	102	2.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105. Diethyl ether [60-29-7]	105	2.414	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108. Tetrahydropyran [142-68-7]	108	3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111. Isobutyl vinyl ether [109-53-5]	111	3.27	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114. Methoxybenzene [100-66-3]	114	3.932	6	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
117. Diphenyl ether [101-84-8]	117	6.449	12	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120. Dibenzyl ether [103-50-4]	120	7.449	12	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
123. Acetaldehyde [75-07-0]	123	1.414	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
126. Crotonaldehyde [123-73-9]	126	2.414	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
129. Isobutylaldehyde [78-84-2]	129	2.27	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
132. 2-Ethylhexanal [123-05-7]	132	4.346	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
135. 2-Butanone [78-93-3]	135	2.27	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
138. 2-Cyclohexen-1-one [930-68-7]	138	3.394	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
141. 2-Hexanone [591-78-6]	141	3.27	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
144. 4-Heptanone [123-19-3]	144	3.808	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
147. 2-Octanone [111-13-7]	147	4.27	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
150. Acetic acid [64-19-7]	150	1.732	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
153. Butyric acid [107-92-6]	153	2.77	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
156. Hexanoic acid [142-62-1]	156	3.77	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
159. Heptanoic acid [111-14-8]	159	4.27	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
162. Ethyl formate [109-94-4]	162	2.414	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
165. Methyl acrylate [96-33-3]	165	2.808	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
168. Isopropyl formate [625-55-8]	168	2.77	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
171. Ethyl acrylate [140-88-5]	171	3.308	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
174. Methyl butyrate [623-42-7]	174	3.308	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
177. Ethyl crotonate [623-70-1]	177	3.808	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
180. Isobutyl acetate [110-19-0]	180	3.626	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
183. Propyl butyrate [105-66-8]	183	4.308	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
186. Methyl benzoate [93-58-3]	186	4.843	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
189. Hexyl acetate [142-92-7]	189	4.77	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
192. Benzyl acetate [140-11-4]	192	5.267	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
195. Isopropyl benzoate [939-48-0]	195	5.698	6	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
198. Benzyl benzoate [120-51-4]	198	7.86	12	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
201. 3-Butenenitrile [109-75-1]	201	2.414	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
204. Pentanenitrile [110-59-8]	204	2.914	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
207. Aziridine [151-56-4]	207	1.5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
210. Pyrrolidine [123-75-1]	210	2.5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
213. Isobutylamine [78-81-9]	213	2.27	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
216. N-Methylpyrrolidine [120-94-5]	216	2.894	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
219. Aniline [62-53-3]	219	3.394	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
222. Diisopropylamine [108-18-9]	222	3.126	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
225. p-Toluidine [106-49-0]	225	3.788	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
228. N,N-Dimethylaniline [121-69-7]	228	4.304	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
231. Diisobutylamine [110-96-3]	231	4.126	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
234. Dipentylamine [2050-92-2]	234	5.414	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
237. N,N-Dibutylaniline [613-29-6]	237	7.361	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
240. 2,4-Dimethylpyridine [108-47-4]	240	3.788	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
243. N-Butylacetamide [1119-49-9]	243	3.77	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
246. N,N-Dibuylacetamide [1563-90-2]	246	5.716	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
249. 1-Nitropropane [108-03-2]	249	2.77	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
252. o-Nitrotoluene [88-72-2]	252	4.715	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
255. 2-Nitrobiphenyl [86-00-0]	255	7.288	12	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
258. Phenyl isocyanate [103-71-9]	258	4.432	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
261. 1-Propanethiol [107-03-9]	261	1.914	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
264. Thiophenol [108-98-5]	264	3.394	6	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
267. 1-Heptanethiol [1639-09-4]	267	3.914	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
270. Dimethyl sulfide [75-18-3]	270	1.414	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
273. 3-Methylthiophene [616-44-4]	273	2.894	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
276. Di-tert-butylsulfide [107-47-1]	276	3.707	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
279. Methyl isothiocyanate [556-61-6]	279	1.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
282. Phenyl isothiocyanate [103-72-0]	282	4.432	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
285. 1-Bromopropane [106-94-5]	285	1.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
288. 2-Methylallyl chloride [563-47-3]	288	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
291. Butyl chloride [109-69-3]	291	2.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
294. 2-Iodobutane [513-48-4]	294	2.27	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
297. Chlorobenzene [108-90-7]	297	3.394	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0

Table 6 (Continued)

Testing (Inputs)

No. Compound [CAS No]	Comp No.	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO
300. Chlorocyclohexane [542-18-7]	300	3.394	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
303. 1-Iodohexane [638-45-9]	303	3.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
306. o-Chlorotoluene [95-49-8]	306	3.805	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
309. o-Fluorotoluene [95-52-3]	**309**	**3.805**	**6**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
312. 1-Bromoheptane [629-04-9]	312	3.914	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
315. 1-Bromooctane [111-83-1]	315	4.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
318. Dichloroacetyl chloride [79-36-7]	318	2.643	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0
321. Ethyl nitrate [625-58-1]	321	2.77	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
324. Propionyl chloride [79-03-8]	324	2.27	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
327. 2,3-Dichloro-1-propanol [616-23-9]	327	2.808	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0
330. 1-Amino-2-propanol [78-96-6]	330	2.27	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
333. 2,3-Butanedione [431-03-8]	333	2.643	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
336. S-Propyl chlorothioformate [13889-92-4]	336	3.27	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0
339. 1,4-Dioxane [123-91-1]	339	3	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
342. Butyl nitrate [928-45-0]	342	3.77	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
345. 1,4-Butanediol [110-63-4]	345	2.914	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
348. 2-Amino-2-methyl-1-propanol [124-68-5]	348	2.561	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
351. Ethyl cyanoacetate [105-56-5]	351	3.808	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
354. Ethyl lactate [97-64-3]	354	3.661	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
357. 4-Methylmorpholine [109-02-4]	357	3.394	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
360. o-Chloronitrobenzene [88-73-3]	360	4.862	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0
363. 2,5-Hexanedione [110-13-4]	363	3.626	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
369. 4-Hydroxy-4-methyl-2-pentanone[123-42-2]	369	3.417	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
372. 2,5-Hexanediol [2935-44-6]	372	3.626	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
375. Triethylenetetramine [112-24-3]	375	4.914	0	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	0	0	0	0	0	0	0	0	0
378. Benzoyl chloride [98-88-4]	378	4.305	6	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
381. Triethylorthoformate [122-51-0]	381	4.846	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
384. 2,5-Dimethoxychlorobenzene [2100-42-7]	384	5.274	6	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
387. Octanoyl chloride [111-64-8]	387	4.77	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
390. Dibutyl disulfide [629-45-8]	390	4.914	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
393. Tripropylene glycol monomethyl ether [20324-33-8]	393	6.558	0	1	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
396. 2-Butoxyethyl salicylate	**396**	**8.253**	**6**	**0**	**1**	**1**	**0**	**0**	**0**	**1**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
399. Diallyl phthalate [131-17-9]	399	8.702	6	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Testing (Target & Results)

No. Compound [CAS No]	Formula	Comp No.	Experimental Data Tb	Experimental Data Tf	ANN Predictions Combined Model Tb	ANN Predictions Combined Model Tf	ANN Predictions Single output Tb	ANN Predictions Single output Tf	PLS Predictions Single Output Tb	PLS Predictions Single Output Tf
3. Pentane [109-66-0]	C5H12	3	**36.1**	**-49.0**	47.6	-28.2	48.0	-26.43	79.3	21.2
6. Cyclohexane [110-82-7]	C6H12	6	**80.7**	**-20.0**	77.4	-10.9	77.3	-9.88	98.6	26.4
9. 2,3-Dimethylbutane [79-29-8]	C6H14	9	**58.0**	**-29.0**	59.4	-21.4	58.5	-19.96	86.9	23.3
12. 2,4-Dimethylpentane [108-08-7]	C7H16	12	**80.6**	**-12.2**	83.6	-7.2	83.7	-6.32	102.7	27.5
15. trans-1,4-Dimethylcyclohexane [2207-04-7]	C8H16	15	**119.4**	**11.1**	115.6	12.0	115.7	12.32	124.5	33.3
18. 2,2,4-Trimethylpentane [540-84-1]	C8H18	18	**99.2**	**-12.0**	97.9	1.3	98.1	1.89	112.3	30.1
21. Dipentene [138-86-3]	C10H16	21	**178.0**	**45.0**	167.2	37.9	155.7	37.60	154.4	41.3
24. Undecane [1120-21-4]	C11H24	24	**195.9**	**60.0**	187.8	57.9	184.7	57.04	178.0	47.6
27. 1-Tetradecene [1120-36-1]	C14H28	27	**256.1**	**110.0**	231.6	88.2	227.8	85.95	214.4	57.4
30. Hexadecane [544-76-3]	C16H34	30	**286.8**	**135.0**	280.1	125.0	282.4	119.33	260.1	89.6
33. Nonadecane [629-92-5]	C19H40	33	**330.6**	**168.0**	324.8	163.4	348.6	150.74	309.4	82.8
36. Styrene [100-42-5]	C8H8	36	**145.2**	**32.0**	142.1	31.7	146.9	36.58	164.2	68.4
39. Ethylbenzene [100-41-0]	C8H10	39	**136.2**	**15.0**	142.1	31.7	146.9	36.58	164.2	68.4
42. Cumene [98-82-8]	C9H12	42	**152.4**	**36.0**	160.4	42.6	165.0	46.69	176.5	71.6
45. Naphthalene [91-20-3]	C10H8	45	**218.0**	**79.0**	204.0	75.1	227.9	87.84	221.6	100.0
48. Isobutylbenzene [538-93-2]	C10H14	48	**172.9**	**55.0**	183.3	56.5	187.4	59.56	192.4	75.9
51. p-Cymen [99-87-6]	C10H14	51	**177.3**	**47.0**	179.1	54.0	183.3	57.18	189.4	75.1
54. Biphenyl [92-52-4]	C12H10	54	**255.3**	**113.0**	249.8	105.7	281.4	120.79	266.1	120.0
57. Anthracene [120-12-7]	C14H10	57	**340.0**	**121.0**	264.8	129.9	323.5	145.60	309.6	139.8
60. Methanol [67-56-1]	CH4O	60	**64.7**	**11.0**	37.3	-11.8	27.1	-8.18	82.7	42.3
63. 1-Propanol [71-23-8]	C3H8O	63	**97.2**	**15.0**	87.3	16.4	85.5	19.55	112.7	50.3
66. 3-Buten-1-ol [627-27-0]	C4H8O	66	**111.7**	**37.8**	113.6	31.5	114.3	33.68	129.2	54.7
69. 2-Butanol [78-92-2]	C4H10O	69	**99.5**	**24.0**	108.1	27.2	108.2	29.61	124.4	53.4
72. Cyclopentanol [96-41-3]	C5H10O	72	**140.9**	**51.0**	138.0	45.7	139.8	47.18	144.9	58.9
75. Isopentyl alcohol [123-51-3]	C5H12O	75	**131.7**	**43.0**	131.8	42.0	133.4	43.72	140.9	57.8
78. 1-Hexanol [11-27-3]	C6H14O	78	**157.5**	**60.0**	163.7	60.9	165.6	61.78	162.0	63.5
81. 4-Methyl-cyclohexanol [589-91-3]	C7H14O	81	**171.0**	**70.0**	181.5	71.6	182.9	72.14	174.3	66.8
84. 1-Octanol [111-87-5]	C8H18O	84	**195.2**	**81.0**	210.1	89.3	210.2	89.33	194.9	72.3
87. 1-Nonanol [143-08-8]	C9H20O	87	**213.1**	**75.0**	231.9	103.2	230.5	102.76	211.3	76.7
90. Phenol [108-95-2]	C6H6O	90	**181.8**	**79.0**	178.0	87.6	184.5	84.28	174.8	91.6
93. p-Cresol [106-44-5]	C7H8O	93	**201.9**	**86.0**	188.7	75.2	184.1	85.32	187.8	95.0
96. o-t-Pentylphenol [3279-27-4]	**C11H16O**	**96**	**282.2**	**103.9**	237.3	106.6	258.9	113.28	246.6	110.8
99. Nonylphenol [25154-52-3]	C15H24O	99	**295.0**	**140.6**	279.0	140.6	336.5	165.76	320.5	130.6
102. Ethyl vinyl ether [109-92-2]	C4H8O	102	**35.7**	**-18.0**	50.6	-16.3	51.5	-21.64	76.4	21.5
105. Diethyl ether [60-29-7]	C4H10O	105	**34.5**	**-45.0**	50.6	-16.3	51.5	-21.64	76.4	21.5
108. Tetrahydropyran [142-68-7]	C5H10O	108	**88.0**	**-20.0**	79.6	-2.8	80.6	-5.10	95.7	26.6
111. Isobutyl vinyl ether [109-53-5]	C6H12O	111	**83.0**	**-9.0**	92.6	4.2	93.2	2.51	104.5	29.0
114. Methoxybenzene [100-66-3]	C7H8O	114	**153.8**	**51.0**	143.0	47.1	145.9	41.74	161.3	68.6
117. Diphenyl ether [101-84-8]	C12H10O	117	**259.0**	**115.0**	264.9	130.0	290.6	134.47	279.0	124.5
120. Dibenzyl ether [103-50-4]	C14H14O	120	**297.0**	**135.0**	297.7	148.7	323.6	152.02	311.9	133.3
123. Acetaldehyde [75-07-0]	C2H4O	123	**20.2**	**-27.0**	18.1	-40.2	20.9	-38.04	43.2	-10.7
126. Crotonaldehyde [123-73-9]	C4H6O	126	**104.0**	**13.0**	71.0	-10.3	79.7	-10.03	76.0	-1.9
129. Isobutylaldehyde [78-84-2]	C4H8O	129	**64.4**	**-18.3**	63.6	-14.6	71.8	-14.08	71.3	-3.1
132. 2-Ethylhexanal [123-05-7]	C8H16O	132	**162.8**	**44.0**	164.4	45.5	171.6	43.97	139.5	15.1
135. 2-Butanone [78-93-3]	C4H8O	135	**79.5**	**-9.0**	75.8	-4.6	76.3	-4.90	98.2	27.2
138. 2-Cyclohexen-1-one [930-68-7]	C6H8O	138	**175.0**	**34.0**	132.6	28.3	135.5	26.65	135.2	37.1
141. 2-Hexanone [591-78-6]	C6H12O	141	**127.2**	**35.0**	128.6	24.7	129.4	23.18	131.1	36.0
144. 4-Heptanone [123-19-3]	C7H14O	144	**144.0**	**49.0**	152.5	40.2	155.0	38.19	148.8	40.7
147. 2-Octanone [111-13-7]	C8H16O	147	**173.5**	**82.0**	173.9	53.3	175.6	50.95	164.0	44.8
150. Acetic acid [64-19-7]	C2H4O2	150	**117.8**	**39.0**	108.2	33.2	102.5	36.15	145.9	81.1
153. Butyric acid [107-92-6]	C4H8O2	153	**163.3**	**77.0**	163.3	65.1	162.9	66.30	180.0	90.2
156. Hexanoic acid [142-62-1]	C6H12O2	156	**205.7**	**104.0**	212.9	94.7	213.0	94.98	212.9	99.0
159. Heptanoic acid [111-14-8]	C7H14O2	159	**223.0**	**112.0**	236.2	109.1	235.6	109.03	229.3	103.4
162. Ethyl formate [109-94-4]	C3H6O2	162	**54.1**	**-20.0**	54.6	-10.1	61.8	-11.64	92.2	28.8
165. Methyl acrylate [96-33-3]	C4H6O2	165	**80.2**	**6.0**	75.5	0.6	81.2	-0.51	105.1	32.3
168. Isopropyl formate [625-55-8]	C4H8O2	168	**67.2**	**-6.0**	73.5	-0.4	79.4	-1.58	103.9	32.0
171. Ethyl acrylate [140-88-5]	C5H8O2	171	**99.5**	**15.6**	101.4	14.1	104.3	13.60	121.6	36.7
174. Methyl butyrate [623-42-7]	C5H10O2	174	**102.5**	**14.0**	101.4	14.1	104.3	13.60	121.6	36.7
177. Ethyl crotonate [623-70-1]	C6H10O2	177	**138.0**	**2.2**	128.5	27.4	125.9	27.63	138.0	41.1
180. Isobutyl acetate [110-19-0]	C6H12O2	180	**116.0**	**18.0**	117.4	22.6	118.2	22.54	132.0	39.5

Table 6. (Continued)

Testing (Target & Results)					ANN Predictions				PLS Predictions	
			Experimental Data		Combined Model		Single output		Single Output	
No. Compound [CAS No]	Formula	Comp No.	Tb	Tf	Tb	Tf	Tb	Tf	Tb	Tf
183. Propyl butyrate [105-66-8]	C7H14O2	183	143.3	37.0	150.8	40.6	146.2	41.55	154.4	45.5
186. Methyl benzoate [93-58-3]	C8H8O2	186	199.5	83.0	196.6	70.6	189.1	67.54	207.0	84.0
189. Hexyl acetate [142-92-7]	C8H16O2	189	171.5	45.0	172.5	52.5	164.1	54.24	169.6	49.6
192. Benzyl acetate [140-11-4]	C9H10O2	192	214.9	90.6	217.9	81.9	208.8	79.07	221.6	87.9
195. Isopropyl benzoate [939-48-0]	C10H12O2	195	219.0	98.9	236.9	92.2	222.7	89.50	235.1	91.5
198. Benzyl benzoate [120-51-4]	C14H12O2	198	323.5	148.0	330.4	150.5	333.4	153.00	341.2	144.3
201. 3-Butenenitrile [109-75-1]	C4H5N	201	119.0	21.0	117.1	15.2	116.2	15.49	125.1	26.6
204. Pentanenitrile [110-59-8]	C5H9N	204	141.3	40.6	142.5	30.0	143.1	29.57	141.6	31.0
207. Aziridine [151-56-4]	C2H5N	207	55.6	-11.1	35.8	-23.0	27.2	-27.70	74.6	27.9
210. Pyrrolidine [123-75-1]	C4H9N	210	88.0	2.8	88.5	6.9	86.6	0.48	107.5	36.7
213. Isobutylamine [78-81-9]	C4H11N	213	68.0	-9.0	74.5	-10.3	73.7	-6.02	93.3	15.6
216. N-Methylpyrrolidine [120-94-5]	C5H11N	216	82.2	-13.9	86.0	-0.6	72.3	-13.18	91.4	14.2
219. Aniline [62-53-3]	C6H7N	219	184.6	70.0	145.7	35.8	151.6	44.14	165.2	59.2
222. Diisopropylamine [108-18-9]	C6H15N	222	84.0	-1.0	120.0	25.3	119.7	18.16	128.1	42.2
225. p-Toluidine [106-49-0]	C7H9N	225	200.0	87.0	165.8	47.5	172.2	54.94	178.2	62.7
228. N,N-Dimethylaniline [121-69-7]	C8H11N	228	193.5	62.8	172.6	54.5	165.2	46.20	172.8	60.3
231. Diisobutylamine [110-96-3]	C8H19N	231	139.5	29.0	167.4	53.9	166.8	46.16	160.9	51.0
234. Dipentylamine [2050-92-2]	C10H23N	234	180.0	51.0	223.1	89.6	220.0	81.13	203.3	62.3
237. N,N-Dibutylaniline [613-29-6]	C14H23N	237	269.5	110.0	300.5	137.5	294.5	122.18	273.9	87.4
240. 2,4-Dimethylpyridine [108-47-4]	C7H9N	240	158.3	37.2	163.2	44.7	152.1	35.78	158.2	41.5
243. N-Butylacetamide [1119-49-9]	C6H13NO	243	235.5	115.6	224.7	117.6	221.2	114.87	235.6	130.4
246. N,N-Dibuylacetamide [1563-90-2]	C10H21NO	246	246.0	107.2	211.9	94.5	196.8	94.73	209.0	95.9
249. 1-Nitropropane [108-03-2]	C3H7NO2	249	131.4	35.6	108.7	15.7	106.8	19.30	118.6	31.5
252. o-Nitrotoluene [88-72-2]	C7H7NO2	252	221.7	106.0	227.2	101.6	229.6	96.80	217.6	82.4
255. 2-Nitrobiphenyl [86-00-0]	C12H9NO2	255	325.0	179.0	338.7	185.0	367.1	180.03	337.2	138.8
258. Phenyl isocyanate [103-71-9]	C7H5NO	258	162.5	55.6	184.4	65.6	191.9	66.83	179.8	59.7
261. 1-Propanethiol [107-03-9]	C3H8S	261	67.7	-20.6	74.2	-14.6	71.6	-12.37	100.9	17.1
264. Thiophenol [108-98-5]	C6H6S	264	169.1	50.6	163.1	41.9	168.4	47.73	184.6	63.9
267. 1-Heptanethiol [1639-09-4]	C7H16S	267	176.9	41.0	174.9	44.4	175.6	44.26	166.6	34.7
270. Dimethyl sulfide [75-18-3]	C2H6S	270	37.3	-36.0	41.5	-20.2	33.0	-16.51	73.5	15.3
273. 3-Methylthiophene [616-44-4]	C5H6S	273	115.4	11.0	119.3	24.2	119.1	25.34	122.2	28.3
276. Di-tert-butylsulfide [107-47-1]	C8H18S	276	151.0	48.0	158.9	47.8	159.0	48.22	148.9	35.4
279. Methyl isothiocyanate [556-61-6]	C2H3NS	279	119.0	32.2	100.8	17.0	98.1	18.09	119.2	36.1
282. Phenyl isothiocyanate [103-72-0]	C7H5NS	282	221.0	87.8	238.3	100.7	242.7	103.31	237.0	92.1
285. 1-Bromopropane [106-94-5]	C3H7Br	285	71.0	25.0	77.0	6.3	71.6	6.55	96.2	33.6
288. 2-Methylallyl chloride [563-47-3]	C4H7Cl	288	72.2	-12.0	59.6	-8.1	62.2	-6.93	82.2	26.8
291. Butyl chloride [109-69-3]	C4H9Cl	291	78.5	-9.4	67.1	-3.8	70.3	-2.89	86.9	28.0
294. 2-Iodobutane [513-48-4]	C4H9I	294	119.0	28.0	128.2	37.4	126.0	39.29	154.9	71.8
297. Chlorobenzene [108-90-7]	C6H5Cl	297	132.0	29.0	132.0	37.7	131.1	43.10	154.1	70.4
300. Chlorocyclohexane [542-18-7]	C6H11Cl	300	143.3	32.0	116.0	24.8	121.3	24.57	119.1	36.7
303. 1-Iodohexane [638-45-9]	C6H13I	303	179.5	61.0	186.1	71.3	186.5	71.88	192.5	81.8
306. o-Chlorotoluene [95-49-8]	C7H7Cl	306	158.9	47.0	153.0	49.8	152.5	54.29	167.6	74.1
309. o-Fluorotoluene [95-52-3]	**C7H7F**	**309**	**114.4**	**12.8**	113.4	21.3	122.0	24.35	136.4	60.3
312. 1-Bromoheptane [629-04-9]	C7H15Br	312	180.0	60.6	176.6	64.6	175.4	62.82	162.0	51.2
315. 1-Bromooctane [111-83-1]	C8H17Br	315	201.0	78.3	199.3	78.6	197.2	76.58	178.4	55.6
318. Dichloroacetyl chloride [79-36-7]	C2HCl3O	318	109.5	66.1	149.6	78.7	170.8	72.93	133.2	50.9
321. Ethyl nitrate [625-58-1]	C2H5NO3	321	87.2	10.0	111.1	24.1	110.8	23.98	115.7	31.8
324. Propionyl chloride [79-03-8]	C3H5ClO	324	79.7	12.0	95.3	19.7	100.5	18.65	105.8	34.0
327. 2,3-Dichloro-1-propanol [616-23-9]	C3H6Cl2O	327	182.0	93.3	170.7	91.0	183.9	90.18	157.2	71.8
330. 1-Amino-2-propanol [78-96-6]	C3H9NO	330	160.0	77.2	140.2	49.2	142.0	53.99	143.1	49.0
333. 2,3-Butanedione [431-03-8]	C4H6O2	333	87.0	26.7	129.9	34.2	136.0	30.31	134.1	37.7
336. S-Propyl chlorothioformate [13889-92-4]	C4H7ClOS	336	155.0	62.8	192.6	86.8	200.2	84.45	165.7	45.6
339. 1,4-Dioxane [123-91-1]	C4H8O2	339	101.4	12.0	81.0	5.4	84.7	-1.00	92.7	26.9
342. Butyl nitrate [928-45-0]	C4H9NO3	342	136.1	36.1	158.8	50.7	157.0	52.31	148.6	40.6
345. 1,4-Butanediol [110-63-4]	C4H10O2	345	230.0	121.1	203.6	105.6	209.2	106.64	195.4	92.6
348. 2-Amino-2-methyl-1-propanol [124-68-5]	C4H11NO	348	165.5	67.2	155.2	57.8	158.1	62.22	152.6	51.6
351. Ethyl cyanoacetate [105-56-5]	C5H7NO2	351	204.8	110.0	195.4	70.5	195.5	69.16	183.8	46.4
354. Ethyl lactate [97-64-3]	C5H10O3	354	154.1	46.0	185.9	83.5	187.7	83.79	183.6	73.5
357. 4-Methylmorpholine [109-02-4]	C5H11NO	357	115.0	23.9	112.2	20.7	99.2	5.64	104.9	18.8
360. o-Chloronitrobenzene [88-73-3]	C6H4ClNO2	360	244.8	127.0	251.6	127.7	248.7	121.85	230.6	90.7
363. 2,5-Hexanedione [110-13-4]	C6H10O2	363	191.4	79.0	178.4	62.5	185.2	57.54	166.4	46.3
369. 4-Hydroxy-4-methyl-2-pentanone[123-42-2]	C6H12O2	369	167.9	58.0	199.4	88.4	203.9	87.06	185.7	70.7
372. 2,5-Hexanediol [2935-44-6]	C6H14O2	372	218.0	110.0	238.1	126.2	243.1	126.29	218.8	98.8
375. Triethylenetetramine [112-24-3]	C6H18N4	375	278.0	135.0	300.3	149.4	308.1	137.72	249.4	63.8
378. Benzoyl chloride [98-88-4]	C7H5ClO	378	196.8	72.0	217.0	90.8	208.1	91.47	207.7	85.7
381. Triethylorthoformate [122-51-0]	C7H16O3	381	143.0	30.0	158.3	49.2	155.5	52.85	150.5	43.4
384. 2,5-Dimethoxychlorobenzene [2100-42-7]	C8H9ClO2	384	237.0	117.2	218.1	112.5	210.5	101.69	210.1	87.5
387. Octanoyl chloride [111-64-8]	C8H15ClO	387	196.0	82.0	214.9	90.9	220.4	87.44	188.0	56.0
390. Dibutyl disulfide [629-45-8]	C8H18S2	390	231.2	93.3	258.3	119.3	257.6	118.03	215.6	48.9
393. Tripropylene glycol monomethyl ether [20324-33-8]	C10H22O4	393	243.3	121.0	281.6	137.1	273.5	153.25	256.6	91.9
396. 2-Butoxyethyl salicylate	**C13H18O4**	**396**	***411.0***	157.2	***294.4***	146.1	304.1	185.28	344.5	142.2
399. Diallyl phthalate [131-17-9]	C14H14O4	399	***298.0***	165.6	***382.1***	166.3	360.9	160.64	346.7	125.6

Figure 3a,b shows the results for the single output models for T_b and T_f, respectively. For these single output models, the network configuration for T_b is 16.5 spread and 36 neurons [26-**36**$_{[16.5]}$-1], the same as the double output model, and for T_f the configuration was 16.8 spread and 26 neurons [26-**26**$_{[16.8]}$-1]. Figure 4a,b shows the results for the double output model for the [26-**36**$_{[16.5]}$-2] configuration.

The average laboratory experimental error for both T_b and T_f is quoted to be around ± 10 °C.[22,23] The results obtained for the validation and testing errors are less than 15 °C (see Table 3a,b). These error levels are close to the stated laboratory absolute error value of 10 °C. As already stated, the prediction errors of the validation and test data provide the true prediction capabilities of the final model. The use of a test set to independently evaluate the final model is therefore very important. The results obtained from the test set provide information related to the model's predictive ability. Further examination of the true predictive capabilities of the final model was performed, by means of an error profile study of 10 random validation and test sets not included in the training process (i.e. random split cross validation). Figure 5 shows the error profiles for the 10 random tests. The open and filled circles (split 1 and 2) have 133 randomly selected samples. This was done by adding the 133 validation and 132 test sets, followed by random rearrangement. The first 133 selected (split1) and the rest, 132 (split2), were then submitted to the optimized model represented by the solid squares in Figure 5. The results show that the error levels for each run have an average of 12 °C and are in the range of 11−13 °C and that the predicted

Table 7. Optimum RBF Network Parameters for Simultaneous Estimation of T_f and T_b[a]

	X	Car	OHal	OHph	-O-	CHO	CO	COOH	-COO-	CN	SH	-S-	NO2	NH2	NH	Nal	Nar	F	Cl	Br	I	CONH	CON	-SO2-	NCS	NCO			
n	W1																										B1	W2'		B2
1	7.788	12.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	2605.11	650.31	-336.53
2	4.966	9.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-488.31	734.29	-86.64
3	6.932	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	821825.40	558106.95	
4	4.788	6.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	1123605.80	463533.56	
5	4.626	0.00	0.00	0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	9814.87	8283.50	
6	3.126	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-11383.13	-5673.56	
7	4.270	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	5992.36	5365.91	
8	7.253	6.00	0.00	1.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-2175099.90	-841085.12	
9	4.787	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.05046	24067.62	23022.93	
10	3.394	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-135371.97	-98350.15	
11	2.414	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	11170.06	9865.07	
12	3.805	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.05046	17569.58	13922.14	
13	2.808	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	13960.20	8658.42	
14	4.121	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.05046	27485.43	20510.67	
15	2.414	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	7287.88	6479.74	
16	1.732	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	4086.55	4800.58	
17	3.394	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-3718.29	-1067.53	
18	3.414	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	9595.51	7686.09	
19	4.698	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	10999.36	19275.35	
20	3.414	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	4348.23	2043.93	
21	2.914	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.05046	15833.66	11979.29	
22	4.414	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	10816.17	5816.07	
23	3.000	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	1626051.60	677784.16	
24	6.753	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.05046	3227.45	6199.79	
25	2.270	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	4796.83	3544.95	
26	4.432	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.05046	4212.24	4233.24	
27	4.432	6.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-544971.90	-326537.53	
28	6.098	6.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	1202909.00	815677.91	
29	3.000	5.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	6566.41	3345.44	
30	1.732	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	2691.53	2434.05	
31	3.270	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-1348.60	-10810.30	
32	7.598	6.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-664243.68	-482776.30	
33	3.805	6.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-2625849.40	-889269.57	
34	9.596	6.00	0.00	0.00	0.00	0.00	0.00	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	367899.70	132964.23	
35	5.410	6.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	4769789.50	1723054.30	
36	4.966	6.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05046	-3939571.20	-1881579.70	

[a] W1: hidden layer weights for each descriptor. W2′: hidden layer weights for the two output targets. B1: bias for hidden layer. B2: bias for output layer.

values for both validation and testing are not due to chance. Considering the wide variety of functionality incorporated into the model and the laboratory error levels for such measurements, together with the size of data set used for the model evaluation, the performance of the RBF is considered to be excellent and reasonable. Examination of the RBF network weight distribution in Figure 6a,b for the single output models shows that all the descriptors contribute to the prediction performance of the network. It is however obvious from the intensities that the aromatic carbons C_{ar} and the first-order molecular connectivity index $^1\chi$ have major contributions, though models based on these two descriptors alone yielded significantly poorer results (not presented here) than the 26 descriptors described above.

In Figure 7 the PLS error profile as a function of number of factors is presented. The results show that the validation and training errors for T_b are significantly lower than T_f values. It is also clear from the error and factor profile for training and validation that the maximum number of factors required for the optimum model is 10 or 11. Beyond these factors no improvement in prediction performance was realized. Figure 8a,b shows the predicted correlation profiles for T_b and T_f, respectively. The PLS results for both T_b and T_f show a significant curvature at lower temperatures (below 100 °C) when comparing experimental and predicted values. The poorer results observed for the optimized PLS model for T_f may be attributed to a substantially nonlinear relationship between the descriptors and T_f. These prediction values are generally poorer than for T_b reflecting the greater nonlinearity for T_f. Because PLS is based on the linear combination of factors the nonlinear behavior could not be modeled efficiently. The accuracy of RBF neural networks for the same set of data confirms the superiority of this modeling approach to PLS. The results clearly indicate that the error profiles for PLS are significantly worse than for RBF networks for both single and double output models, as summarized in Table 3. Tables 4−6 show all the data used for the modeling, including NN and PLS results for each compound. The NN weight distribution for the simultaneous prediction of T_f and T_b has been provided in Table 7. These values however requires Matlab[31] and the associated Neural Network Toolbox. Details of how to use these parameters are provided in the Appendix. W1 and W2′ are the hidden layer weights for each of the 26 descriptors and two output layers, respectively. B1 and B2 are the biases for the hidden and output layers. As for the single target models $^1\chi$ and C_{ar} clearly have the greatest effect, but there are no redundant functional groups and neurons.

CONCLUSIONS

The results obtained in this paper demonstrate that it is possible to generate a robust single network capable of simultaneous estimation of T_f and T_b using a nonhomogeneous functional group data set. The inputs required for these estimations were based solely on numerical coding of the molecule and can be readily generated if the molecular formula is known. The success of this neural model is the result of robust optimization strategy via the biharmonic response surface analysis, followed by further evaluation using a random split cross-validation analysis. A multioutput single model may not necessarily be a significant advantage for the type of data examined in this work; however, in applications where simultaneous classification of complex systems are required, the optimization strategy used in this work will be very advantageous. Typical application areas are, for example, medical diagnosis where classification into groups is the goal, or very portable embedded electronic systems where a single network capable of multidecision output, will save energy, space/memory, and analysis time. The realization of a final working model in less than 10 min on a 166 MHz PC with 32 MB RAM is a significant improvement in modeling such a QSPR systems, since backpropagation training and optimization with advance learning schemes still requires several hours of training though an explicitly optimized model cannot be guaranteed. It is also clear from the PLS results that the neural models have superior modeling and prediction capabilities.

**APPENDIX

Symbols and formulas used in figures: σ, spread; **n**, number of neurons in hidden layer; and r, regression correlation coefficient,

The average absolute error, AE and the standard error, SE are given by

$$\mathrm{AE} = \sum ||X_t - X_p||/n$$

$$\mathrm{SE} = \sqrt{(((\sum X_t - X_p)^2/n))}$$

where X_t is the experimental value, X_p is the predicted value, n is the number of samples, and ||.|| is the norm.

MATLAB function for simultaneous prediction of T_f and T_b

[Predicted] = simurb(Input,W1,B1,W2′,B2)

W1, B1, W2, are B2 are provided in Table 7. The superscript ′ is the transpose of the matrix or vector. The Input is a one column vector (Descriptors) as indicated in Table 2, and the Predicted output is also a one column two row vector, where rows 1 and 2 are T_b and T_f, respectively.

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