

# QSPR Modeling of Soil Sorption Coefficients ( $K_{OC}$ ) of Pesticides Using SPA-ANN and SPA-MLR

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A quantitative structure-property relationship (QSPR) study was conducted to predict the adsorption coefficients of some pesticides. The successive projection algorithm feature selection (SPA) strategy was used as descriptor selection and model development method. Modeling of the relationship between selected molecular descriptors and adsorption coefficient data was achieved by linear (multiple linear regression; MLR) and nonlinear (artificial neural network; ANN) methods. The QSPR models were validated by cross-validation as well as application of the models to predict the  $K_{OC}$  of external set compounds, which did not contribute to model development steps. Both linear and nonlinear methods provided accurate predictions, although more accurate results were obtained by the ANN model. The root-mean-square errors of test set obtained by MLR and ANN models were 0.3705 and 0.2888, respectively.

KEYWORDS: Quantitative structure-activity relationship; soil sorption coefficients; successive projection algorithm; artificial neural network

# INTRODUCTION

The widespread use and distribution of pesticides, chemicals released deliberately and in large quantities into the environment, are of great relevance today. The potential for adverse consequences of pesticides, such as environmental impact on the quality of water and wildlife habitats, has led to the development of detailed analyses of potential environmental hazards associated with the use of these compounds (1-3). Knowledge of pesticide environmental behavior, such as adsorption to soil, leaching to groundwater, and volatility in the atmosphere, is of primary concern for an accurate assessment of the risk to the environment and humans. Pesticide distribution and fate in various environmental media and compartments are strongly influenced by the inherent properties of the compounds themselves, particularly by basic physicochemical properties such as solubility in water, vapor pressure (VP), and partitioning coefficients between organic matter (in soil or sediment) and water. In the assessment of pesticide environmental behavior it is important to understand the properties that control pesticide partitioning tendencies. Recently, some molecular modeling methods based on widespread quantitative structure-property/activity relationships (QSPR/QSAR) techniques have found their place as important tools for chemists (4, 5).

The reliable estimation of soil sorption coefficients ( $K_{\rm OC}$ ) for organic pesticides plays a fundamental role in agriculture, especially for describing the pollution impact of the pesticides and their tendency for biodegradation. This partition coefficient represents a measure of the retaining of a chemical by the organic matter of soils and sediments through a wide variety of possible intermolecular interactions (6, 7). Nowadays, fewer than 300 chemicals have measured  $K_{\rm OC}$  values, and little information is available on the sorption behavior of their metabolites (8). Clearly, the prediction of the  $K_{\rm OC}$  parameter for a wide number of chemical structures is very convenient for application in risk assessment.

A generally accepted remedy to surmount the lack of availability of experimental data in contemporary chemistry is the application of quantitative structure-property relationships (QSPR) analysis (9), in the present case to obtain adequate predictions for soil sorption coefficients. The ultimate role of the different formulations of the QSPR theory is to suggest mathematical models for estimating relevant end points of interest, especially when these cannot be experimentally determined for some reason. These studies simply rely on the assumption that the structure of a compound determines the physicochemical properties it manifests. The molecular structure is therefore translated into the so-called molecular descriptors through mathematical formulas obtained from several theories, such as chemical graph theory, information theory, and quantum mechanics (10, 11). There exist more than a thousand theoretical descriptors available in the literature, and one usually faces the

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problem of selecting those that are the most representative for the property under consideration. In this investigation, we introduce the successive projections algorithm (SPA) (12) as a feature selection, due to its ability in solving the descriptor selection problems in QSPR model development.

SPA is a technique specifically designed to select subsets of variables with small collinearity and to improve the conditioning of multiple linear regression (MLR) models. This algorithm was originally proposed for wavelength selection in spectroscopic data sets, especially under conditions of strong spectral overlapping (12). MLR models obtained by using SPA have been shown to be superior, in terms of prediction ability, to full-spectrum partial least squares (PLS) models in a variety of applications, including UV-vis (12–15), ICP-OES (16), FT-IR (17), and NIR spectrometry (17–19). SPA has also been successfully employed in various classification studies (20, 21).

SPA comprises three phases (22). Initially, the algorithm builds candidate subsets of variables on the basis of a collinearity minimization criterion. Such subsets are constructed according to a sequence of vector projection operations applied to the columns of the matrix of available predictor data. In the second phase, the best candidate subset is chosen according to a criterion that evaluates the prediction ability of the resulting MLR model, such as the root-mean-square error obtained in a validation set (23). In the third phase, the selected subset is subjected to an elimination procedure to determine whether any variables can be removed without significant loss of prediction ability. Each of these phases is explained in detail elsewhere (24).

Although SPA was initially designed for use with MLR models, it may be worth investigating whether it could be employed with different modeling techniques. In the present paper, the variables selected by SPA will be used to build MLR and artificial neural network (ANN) models.

## MATERIALS AND METHODS

**Data.** Experimental soil sorption coefficient  $(K_{OC})$  data of the 124 pesticides were used in this work (25). A QSPR model for the estimation of the soil sorption coefficient of pesticides is established in the following six steps: the molecular structure input and generation of the files containing the chemical structures is stored in a computer-readable format; quantum mechanics geometry is optimized with a semiempirical (AM1) method; structural descriptors are computed; structural descriptors are selected; and the structure-K<sub>OC</sub> model is generated by MLR, ANN, and statistical analysis. The names of these compounds and their experimental and calculated values by ANN and MLR methods are shown in Table 1. As can be seen, this set contains 124 soil sorption coefficients ( $K_{OC}$ ) data of pesticides. The data set was split into training, validation, and test sets. The training set of 62 compounds, with log  $K_{OC}$  values ranging from 0.301 to 6.000, was used to construct the model. The validation set of 31 compounds, with log  $K_{OC}$  values ranging from 0.531 to 5.00, was used to prevent overtraining/overfitting of the ANN model. The test set of 31 compounds, with  $K_{OC}$  values ranging from 0.301 to 4.204, was used as an external set to evaluate the predictive ability of the model.

**Descriptor Generation and Screening.** For calculating  $K_{OC}$ , we have used the well-known EPI  $K_{OC}$  estimation tool (26). The soil sorption coefficients ( $K_{OC}$ ) of solutes are related to some of their structural, electronic, and geometric properties. The value of these properties can be encoded quantitatively by numerical values named molecular descriptors. These molecular parameters are to be used to search for the best QSPR model of the soil sorption coefficients. The 2D structures of the molecules were drawn using Hyperchem 7 software (27). The final geometries were obtained with the semiempirical AM1 method in the Hyperchem program. The molecular structures were optimized using the Polak–Ribiere algorithm until the root-mean-square gradient was 0.001 kcal mol<sup>-1</sup>. The resulting geometry was transferred into the Dragon program package, which was developed by a Milano chemometrics and QSPR group (28), to calculate 1457 descriptors in constitutional, topological, geometrical, charge, GETAWAY (Geometry, Topology and Atoms-Weighted Assembly), WHIM (Weighted Holistic Invariant Molecular descriptors), 3D-MoRSE (3D-Molecular Representation of Structure based on Electron diffraction), molecular walk count, BCUT, 2D autocorrelation, aromaticity index, randic molecular profile, radial distribution function, functional group, and atom-centered fragment classes.

It is worth mentioning that in the first preselected analysis we removed 647 descriptors because many of them included zero or other constant/ near-constant values and did not have enough information of structure. On the other hand, to decrease the redundancy existing in the descriptor data matrix, the correlation coefficient *r* of the descriptors with each other was examined and the collinear descriptors (with r > 0.9) were removed.

Upon application of SPA, seven descriptors were selected for model building. These descriptors were as follows: H total index/weighted by atomic polarizabilities (HTp); Moran autocorrelation lag-6/weighted by atomic Sanderson electronegativities (MATS6e); third-component symmetry directional WHIM index/weighted by atomic van der Waals volumes (G3v); 3D-MoRSE-signal05/weighted by atomic masses (Mor05m); first-component symmetry directional WHIM index/weighted by atomic masses (G1m); Moran autocorrelation lag-4/weighted by atomic polarizabilities (MATS4p); and highest eigenvalue n.2 Burden matrix/weighted by atomic masses (BEHm2).

The first selected descriptor is H total index/weighted by atomic polarizabilities (HTp), which is a GETAWAY descriptor. GETAWAY tries to match the 3D molecular geometry provided by the molecular influence matrix and atom relatedness by topology with chemical information by using different atomic weighting schemes (unit weights, mass, polarizability, electronegativity).

The molecular influence matrix **H** is defined by

$$\mathbf{H} = \mathbf{M}(\mathbf{M}^T \mathbf{M})\mathbf{M}^T \tag{1}$$

where **M** is the molecular matrix. The resultant  $A \times A$  matrix is invariant to rotation of the molecular coordinates. The diagonal elements  $h_v$  are termed leverages and represent the influence of each atom in determining the shape of the molecule. Each off-diagonal element  $h_v$  represents the degree of accessibility of the  $j^{\text{th}}$  atom to interactions with the  $i^{\text{th}}$  atom (29).

The second and third descriptors that were selected for the QSPR model were Moran autocorrelation lag-6/weighted by atomic Sanderson electronegativities (MATS6e) and Moran autocorrelation lag-4/weighted by atomic polarizabilities (MATS4p). These descriptors are 2D autocorrelation descriptors. The structural variables introduced by Moran correspond to bidimensional autocorrelations between pairs of atoms in the molecule and are also defined to quantify the contribution of a considered atomic property to the analyzed property. These can be readily calculated, that is, by summing products of terms including the atomic weights for the terminal atoms in all of the paths of a prescribed length. For the case of MATS6e, the path connecting a pair of atoms has a length of 6 and involves the atomic Sanderson electronegativities as weighting scheme.

The next selected descriptors were third-component symmetry directional WHIM index/weighted by atomic van der Waals volumes (G3v) and first-component symmetry directional WHIM index/weighted by atomic masses (G1m), which are a kind of WHIM descriptor. WHIM descriptors are molecular descriptors based on statistical indices calculated on the projection of the atoms along principal axes. Also, WHIM descriptors are built in such a way as to capture relevant molecular 3D information regarding molecular size, shape, symmetry, and atom distribution with respect to invariant reference frames. The algorithm consists of performing a principal component analysis on the centered Cartesian coordinates of molecules by using a weighted covariance matrix obtained from different weighting schemes for atoms

$$S_{jk} = \frac{\sum_{i=1}^{A} w_i(q_{ij} - \overline{q_j})(q_{jk} - \overline{q_k})}{\sum_{i=1}^{A} w_i}$$
(2)

where  $S_{jk}$  is the weighted covariance between the  $j^{\text{th}}$  and  $k^{\text{th}}$  atomic coordinates, A is the number of atoms,  $w_i$  the weight of the  $i^{\text{th}}$  atom,  $q_{ij}$ 

Table 1. Data Set with Experimental and Calculated Soil Sorption Coefficients (Log  $K_{OC}$ )<sup>a</sup>

1         acaphale         0.031         0.191         0.234         1.238         63         alkicab         0.903         1.278         1.468         3.277         2.568           3         intazne         2.003         1.327         2.104         5.227         66         bennoxalin         1.344         1.468         2.492         2.492           5         broncal         1.505         1.468         1.449         2.625         66         belnox         3.030         3.179         2.898         2.492           6         catholizan         1.344         2.468         2.444         2.646         66         catholizan         3.417         1.327         1.328         1.271         1.327         1.328         1.241         1.248         1.241         1.248         1.241         1.248         1.241         1.248         1.241         1.248	no.	compound	$\log K_{\rm OC}$ (exptl)	ANN	MLR	EPI	no.	compound	$\log K_{\rm OC}$ (exptl)	ANN	MLR	EPI
2         atkrim         3.699         1.827         2.018         2.874         6.65         amazine         2.944         2.644         2.177         2.585           4         berndicasth         2.766         2.510         2.104         2.167         6.5         bernacin         1.944         1.683         1.777         2.745           6         captan         2.104         2.668         2.841         6.6         cathetamide         1.946         1.966         1.757         2.77           7         cartholution         1.332         2.371         3.401         3.161         70         critorization         3.667         3.171         2.014         2.838         2.	1	acephate	0.301	0.819	0.324	1.338	63	aldicarb	0.903	1.376	1.668	3.371
3         atrazne         2.039         1.227         2.104         5.152         bencazin         1.344         1.848         1.278         1.137           5         bromaal         1.505         1.448         1.349         5.025         67         bulylate         3.802         3.116         2.848         2.842           6         catroluran         1.342         2.131         2.100         1.886         69         catrolurande         3.142         3.203         7.77         3.233         2.787         3.233         2.787         3.233         2.787         3.233         2.787         3.233         2.788         3.401         3.161         0.66         catroluroptica         3.112         3.020         2.441         2.472         2.772         1.347         1.505         1.881         2.164         2.145         1.444         1.444         1.444         1.444         1.444         1.444         1.444	2	aldrin	3.699	3.397	3.784	3.494	64	anilazine	2.344	2.464	2.177	2.558
4         berndicamb         2.766         2.810         2.104         1.512         66         bitnox         3.833         3.815         3.816         3.816         3.816         3.816         3.816         1.485         1.485           6         captan         2.104         2.266         2.441         66         cabiconab         1.77         3.237         3.237         3.401         3.161         70         chionphilos         3.607         3.112         3.00         4.84         2.788         2.782         71         cybernethin         3.007         4.84         2.458         2.478         72         71         cybernethin         3.007         3.161         73         dinacto         2.778         2.838         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.868         2.878         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868         3.868	3	atrazine	2.093	1.827	2.018	2.267	65	benazolin	1.344	1.683	1.278	1.137
5         bromaal         1.465         1.448         5.25         67         bubyate         3.042         3.946         3.947         1.777         1.277           7         carbofuran         1.342         2.113         2.100         1.386         69         chioromeb         3.217         3.237         3.238         2.382         2.788           8         chiorotholn         3.302         3.717         2.782         7.1         cypermethra         5.000         1.849         4.5	4	bendiocarb	2.756	2.610	2.104	1.512	66	bifenox	3.383	3.150	2.889	2.922
6         captan         2.104         2.866         2.841         2.648         68         catebaranie         1.944         1.959         1.777         1.274           8         chlorothaloni         3.932         3.771         3.401         3.161         70         chlorothaloni         3.897         2.887         2.887         2.887         2.887         2.887         2.887         2.887         2.887         2.881         1.881         2.881         2.881         1.881         2.881         2.881         1.881         2.881         2.881         2.881         1.881         2.881         1.881         2.881         1.881         2.881         1.881         2.881         2.881         3.881         8.81         1.881         2.881         2.881         3.881	5	bromacil	1.505	1.485	1.349	5.025	67	butylate	3.602	3.116	3.415	1.493
7         cataboluram         1.342         2.113         2.101         1.386         68         ohkoraphilos         3.217         3.238         2.288           9         chiorsulturon         1.602         1.879         2.982         2.78         2.387         7         1.344hohopropene         5.000         4.549         4.543         2.388           10         diziono         2.444         2.742         2.876         7         1.344hohopropene         1.505         1.818         1.848         1.546         2.484         3.484           11         diction         2.457         2.868         2.768         3.484         1.207         7         FEPTC         2.082         2.311         2.544           11         edimorphos         2.004         1.715         2.278         1.574         7         1.600apopP         3.620         2.181         2.445           15         ethopcophos         2.004         1.511         1.755         2.017         7         9         phychostale         2.223         2.212         2.283         3.162           16         fenzopaton         1.308         3.463         2.789         80         methodihohomethum         3.31         2.464	6	captan	2.104	2.656	2.841	2.648	68	carbetamide	1.946	1.959	1.767	1.274
8         chicottalanii         3.932         3.771         3.401         3.161         7.0         chicotynics         3.817         3.112         3.09         2.847           10         diaziron         2.434         2.724         2.875         2.75         7.2         1.3-dichicorpopene         1.501         1.861         2.162         2.434           11         dichicorpo         3.000         2.445         2.447         7.44         disulforon         2.783         2.838         2.890         2.393           12         dimethoate         3.011         1.754         2.284         2.170         7.5         EPCC         2.082         2.370         3.824           15         efferoxycath         3.033         3.042         2.787         2.781         7.74         7.76         efferoxapport         2.245         3.171         1.000           16         efferoxycath         3.033         1.611         7.257         2.716         7.6         efferoxapport         2.333         1.610         1.682         3.991         9.0         iprodine         2.873         3.814         2.182         2.246         2.811         1.844         1.843         1.866         2.883         8.100 <td< td=""><td>7</td><td>carbofuran</td><td>1.342</td><td>2.113</td><td>2.100</td><td>1.386</td><td>69</td><td>chloroneb</td><td>3.217</td><td>3.237</td><td>3.283</td><td>2.788</td></td<>	7	carbofuran	1.342	2.113	2.100	1.386	69	chloroneb	3.217	3.237	3.283	2.788
9         ehhorsulturon         1.602         1.879         2.882         71         oppermethy         5.05         1.459         1.4612         2.884           11         dichlorprop         3.000         2.454         2.457         72         1.31dhlorprope         1.595         1.816         2.169         2.398         2.680         2.398         2.680         2.398         2.680         2.398         2.680         2.398         2.680         2.398         2.370         3.58           12         diuron         2.657         2.768         3.243         1.207         75         EPTC         2.084         2.311         2.544         2.481         1.444           15         ethorprophos         2.004         2.728         3.738         78         Tentomorp-78         3.68         2.316         2.481         1.441           16         fenzorpath         2.004         2.728         3.217         79         glyphosata         2.202         2.455         1.600           18         feazone         1.731         1.611         1.752         2.787         7.80         81         methomon         2.612         2.248         2.317         1.600           19         mobasinin	8	chlorothalonil	3.932	3.771	3.401	3.161	70	chlorpyrifos	3.697	3.112	3.09	2.647
10         diakinom         2.434         2.73         2.75         72         1.3-dirikiopropen         1.061         1.268         1.564         3.438           12         dimethoate         1.301         1.754         2.268         1.000         76         EPTC         2.062         2.238         2.303         3.268           14         eeforwalente         3.724         3.830         4.078         2.716         76         ethotmssate         2.170         2.466         2.311         2.544           15         ethocyophos         2.004         1.715         2.276         778         floomastate         2.176         78         floomastate         2.178         2.381         1.611         1.513         1.611         1.755         2.276         3.034         2.73         1.000           19         isolenphos         2.776         7.308         8.168         2.688         81         inturon         2.567         2.738         3.034         2.73         1.030           19         isolenphos         2.776         7.308         3.168         2.688         81         inturon         2.57         2.738         3.102         4.53           10         methino-methy <t< td=""><td>9</td><td>chlorsulfuron</td><td>1.602</td><td>1.879</td><td>2.390</td><td>2.362</td><td>71</td><td>cypermethrin</td><td>5.000</td><td>4.549</td><td>4.612</td><td>2.638</td></t<>	9	chlorsulfuron	1.602	1.879	2.390	2.362	71	cypermethrin	5.000	4.549	4.612	2.638
11       dichloprop       3.000       2.454       2.477       1.463       73       diculon       2.778       2.268       2.249       2.390       2.328         13       diuron       2.657       2.768       3.243       1.007       75       EPTC       2.028       2.239       2.370       3.284         15       eefervolatelete       3.747       3.264       1.574       77       fencourp.P       3.64       2.3176       2.813       1.444         16       fencovach       3.000       3.042       2.728       3.778       7.8       fencourp.P       3.63       2.316       2.453       1.716         16       fencovach       3.000       3.042       2.728       3.778       7.8       fencourp.P       3.634       2.317       1.600         18       fexatome       1.732       1.661       1.829       3.931       8.01       feuron       2.528       1.629       3.33       2.191       2.030       3.44       1.990       phosato       2.432       2.818       3.046       4.253       1.000       7.9       phosato       3.433       3.245       3.106       1.000       3.302       2.295       1.101       1.177       3.433 <t< td=""><td>10</td><td>diazinon</td><td>2.434</td><td>2.724</td><td>2.873</td><td>2.375</td><td>72</td><td>1,3-dichloropropene</td><td>1.505</td><td>1.861</td><td>2.106</td><td>2.149</td></t<>	10	diazinon	2.434	2.724	2.873	2.375	72	1,3-dichloropropene	1.505	1.861	2.106	2.149
12         dimembate         1.301         1.754         2.268         1.268         2.680         2.890         2.890         2.890         2.890         2.890         3.828           14         esfervalerele         3.724         3.830         4.078         2.716         76         etholymesate         2.170         2.461         2.811         2.848           15         ethopryphos         3.004         3.72         2.776         778         floometuron         2.020         2.456         2.871         1.446           16         fenoxporph         3.000         3.042         2.772         3.038         816         inuron         2.657         2.73         1.000           19         iodenphos         2.771         2.708         828         816         inuron         2.657         2.73         1.000           19         iodenphos         2.751         2.710         2.386         81         inuron         2.697         2.323         2.132         2.303         3.164         4.648         4.428         3.044         4.55         3.053         3.110         4.65         3.054         4.640         4.428         4.015         4.640         4.421         4.255         4.110 <td>11</td> <td>dichlorprop</td> <td>3.000</td> <td>2.454</td> <td>2.457</td> <td>1.843</td> <td>73</td> <td>dinoseb</td> <td>1.591</td> <td>1.428</td> <td>1.564</td> <td>3.387</td>	11	dichlorprop	3.000	2.454	2.457	1.843	73	dinoseb	1.591	1.428	1.564	3.387
diuron         2.657         2.768         3.243         1.207         75         EPTC         2.082         2.233         2.470         3.582           15         eefhognophos         2.004         1.715         2.276         1.574         77         fenoxaprop-P         3.652         3.716         2.616         1.656           16         fenoxaprop-1         1.531         1.611         1.755         2.017         79         olyphosate         2.223         2.220         2.455         3.167           18         hexacnnen         1.732         1.606         1.829         2.384         81         methicantion         2.212         2.238         2.176         2.56         1.677           21         methicanthon         2.253         3.238         2.384         84         parathion         3.628         3.243         1.248         3.646         4.287         3.030         3.032         2.232         2.128         2.55         1.679           22         methicanthon         2.243         2.437         2.333         2.211         2.061         8.5         prioration         3.689         3.243         3.1246           23         parathion-methyi         3.030         3.036	12	dimethoate	1.301	1.754	2.286	1.000	74	disulfoton	2.778	2.638	2.690	2.399
14         esternalerate         3.724         3.830         4.078         2.716         76         etholumestate         2.707         2.488         2.311         2.543           15         etholyophos         3.000         3.042         2.792         3.778         78         flourophor         2.202         2.454         2.653         3.167         2.816         3.168         2.817         79         glophostate         2.220         2.456         3.167         2.55         3.167         2.58         3.169         3.463         2.783         3.091         glophostate         2.220         2.455         3.167         2.58         3.169         3.463         2.783         3.284         2.283         1.29         2.280         2.55         1.070         2.382         2.222         2.285         1.10         2.465         3.233         2.211         2.261         8         parathion         3.684         3.044         2.209         65         phorate         3.000         2.905         2.305         1.10         3.022         2.235         1.030         2.205         1.11         2.107         2.448         2.301         1.435         2.445         2.301         1.435         2.445         2.445         2.441	13	diuron	2.657	2.768	3.243	1.207	75	EPTC	2.082	2.233	2.370	3.528
15       ethospophos       2.004       1.715       2.276       1.574       77       tenospopho       2.002       2.148       2.016       1.686         17       fluoroxpyr       1.531       1.611       1.755       2.017       79       glyphosate       2.223       2.220       2.455       3.173       1.000         19       isolerxphos       2.778       3.038       3.165       2.838       81       inuron       2.247       2.232       2.19       2.280       2.155       1.070         20       malathion       3.255       3.059       3.489       2.489       82       metholathio       2.242       2.18       3.046       4.682         21       methocath       2.751       2.710       2.383       82       metholathion       2.249       2.818       3.046       4.642         23       parathion-methyl       3.030       3.023       4.122       2.061       86       pinorthos       1.030       3.032       2.923       2.452       1.030       3.032       2.917       2.676       3.044       3.45       4.064       3.047       1.917       1.912       1.711       2.177       7.718       2.917       3.676       91       pinothio	14	esfenvalerate	3.724	3.830	4.078	2.716	76	ethofumesate	2.170	2.486	2.311	2.544
16       tenoxycarb       3.000       3.042       2.782       3.778       78       funcaturon       2.000       2.148       2.201       2.456       3.187         18       hexazinone       1.732       1.006       1.829       3.991       80       iprodione       2.279       3.034       2.78       3.034       2.78       3.034       2.78       3.034       2.78       3.034       2.78       3.034       2.78       3.04       2.78       3.044       2.78       3.04       4.72       2.98       2.85       1.97       2.71       2.210       2.58       1.97       2.71       2.71       2.70       2.38       3.16       4.68       2.23       parathion-methyl       2.303       2.31       2.241       2.80       6.6       phorat       3.000       2.02       2.385       1.110       3.000       3.032       2.232       2.426       2.80       1.110       3.000       2.005       2.385       1.110       3.000       2.025       2.385       1.110       3.000       2.025       2.385       1.110       3.000       2.026       2.385       1.110       3.000       3.02       2.262       2.56       1.57       2.56       1.57       1.56       1.511       <	15	ethoprophos	2.004	1.715	2.276	1.574	77	fenoxaprop-P	3.652	3.716	2.813	1.484
17       fluoroxpyr       1.531       1.611       1.755       2.017       79       glyphosate       2.223       2.220       2.455       3.167         19       isofenphos       2.778       3.008       3.991       80       ipor       2.597       2.203       2.129       2.260         0       malathion       2.251       2.771       2.033       2.212       2.268       3.044       4.223       2.281       3.044       4.223         21       methularion       1.544       1.403       1.896       2.384       84       parathion       2.463       3.423       3.31       2.466         22       parathion-methyl       2.373       2.211       2.061       85       phorate       3.000       2.902       2.151       2.160       2.902       2.903       3.012       2.244       2.155       1.171       2.164       2.160       2.397       2.160       3.003       2.242       2.155       1.177       2.178       2.164         25       procohar       1.747       2.181       2.660       2.379       9.04       subinor       1.892       1.717       2.178       2.177       2.178       3.069       subinon       1.813       1.363	16	fenoxycarb	3.000	3.042	2.792	3.578	78	fluometuron	2.000	2.148	2.081	1.686
18         hexazinone         1.722         1.606         1.829         3.991         80         iprodione         2.679         3.034         2.73         1.000           20         malethion         3.255         3.069         3.483         2.786         82         methidahion         2.242         2.281         2.55         1.079           21         methicathic         2.247         2.338         2.238         83         methicathic         2.242         2.818         3.046         4.282           22         methication-methyl         2.373         2.332         2.211         2.601         85         phronethyl         3.000         2.905         2.685           24         phosolone         4.255         3.924         4.122         2.209         86         priopacitol         2.937         2.767         1.710         4.74         4.800           26         propanil         2.173         2.214         2.870         1.839         photocation         1.882         2.711         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171	17	fluoroxypyr	1.531	1.611	1.755	2.017	79	glyphosate	2.223	2.220	2.455	3.187
19         isofenphos         2.778         3.088         3.165         2.838         2.19         Land         2.55         1.679           21         methicath         2.751         2.710         2.388         2.385         83         metolachior         2.243         2.2818         3.046         4.628           22         metsulturon         1.544         1.493         1.896         2.384         84         parathion         3.693         3.423         3.31         2.466           23         parathion-methyl         2.373         2.231         2.204         65         phorate         3.000         2.905         1.103         86         propicon-nethyl         3.032         2.242         2.466           25         procolinaz         3.864         3.645         1.047         1.803         88         propiconzole         2.997         3.170         3.474         3.250           26         procolnari         6.173         2.244         2.870         1.903         8.81         propiconzole         2.997         3.477         2.476           29         thidemorph         3.080         2.951         2.646         2.707         94         achichor         2.462         2.547 <td>18</td> <td>hexazinone</td> <td>1.732</td> <td>1.606</td> <td>1.829</td> <td>3.991</td> <td>80</td> <td>iprodione</td> <td>2.679</td> <td>3.034</td> <td>2.73</td> <td>1.000</td>	18	hexazinone	1.732	1.606	1.829	3.991	80	iprodione	2.679	3.034	2.73	1.000
20         meltihoarb         2.255         3.059         3.493         2.789         82         methidathion         2.212         2.289         2.55         1.070           21         methiocarb         2.761         2.388         2.938         methiochrin         3.648         3.423         3.31         2.468           22         parathon-methyl         2.373         2.233         2.211         2.061         B5         phorath         3.000         2.905         2.365         1.110           24         phosalone         4.255         3.923         4.122         2.209         86         phirmiphos-methyl         3.000         3.032         2.923         2.456           25         proponur         1.477         1.931         2.057         2.739         88         sulfometuron         1.832         2.244         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.171         2.172         2.753         2.677         2.779         9         9         terbutyn         2.81         2.646         2.707         9         2.614         1.767           23         amitore         2.079         2.581 <t< td=""><td>19</td><td>isofenphos</td><td>2.778</td><td>3.038</td><td>3.165</td><td>2.638</td><td>81</td><td>linuron</td><td>2.597</td><td>2.323</td><td>2.129</td><td>2.260</td></t<>	19	isofenphos	2.778	3.038	3.165	2.638	81	linuron	2.597	2.323	2.129	2.260
21       methiocarb       2.751       2.710       2.358       2.835       83       metolachlor       2.243       2.818       3.046       4.263         22       metsulfuron       1.544       1.443       1.896       2.834       4.8       parathion       3.000       2.905       2.365       1.110         24       phosalone       4.255       3.923       4.122       2.099       86       primiphos-methyl       3.000       2.905       2.365       1.406         25       prochoraz       3.864       3.412       2.209       86       primiphos-methyl       3.002       2.957       2.711       4.474       4.905         27       propoour       1.477       1.931       2.057       2.733       98       sulfometuron       1.822       2.711       2.171       2.171       2.474       2.836       2.957       2.576         29       thifensulfuron       1.650       2.059       3.378       91       thiriam       0.351       0.464       0.844       5.250         30       tridemorph       3.308       2.951       3.230       2.216       2.646       2.707       94       actintorfan       2.427       2.545       1.156       1.575	20	malathion	3.255	3.059	3.493	2.789	82	methidathion	2.212	2.289	2.55	1.079
22         metalufurion         1.544         1.493         1.896         2.384         64         parathion         3.698         3.423         3.211         2.465           23         parathion-methyl         3.000         2.365         1.110           24         phosalone         4.255         3.923         4.121         2.209         86         piropiphos-methyl         3.000         3.032         2.284         2.613           25         proponitoraz         3.864         3.645         4.047         1.800         87         proponizole         2.957         3.170         3.474         3.255           26         proposur         1.477         1.931         2.057         2.739         89         sulfometuron         1.892         1.711         2.177         2.77           29         thidensulfuron         1.653         1.636         2.039         3.378         91         thiriam         0.531         0.846         2.807           31         tidemorph         3.308         2.451         2.246         2.707         94         actiluorfen         2.052         2.256         1.571           32         alachior         2.105         2.116         1.965         2.278 <td>21</td> <td>methiocarb</td> <td>2.751</td> <td>2.710</td> <td>2.358</td> <td>2.935</td> <td>83</td> <td>metolachlor</td> <td>2.243</td> <td>2.818</td> <td>3.046</td> <td>4.628</td>	21	methiocarb	2.751	2.710	2.358	2.935	83	metolachlor	2.243	2.818	3.046	4.628
23         parathion-methyl         2.373         2.233         2.211         2.061         85         pinotaci         3.000         2.905         2.365         1.110           24         phosalone         4.255         3.923         4.12         2.204         86         pinipinbos-methyl         3.000         3.022         2.232         2.466           25         propanil         2.173         2.214         2.870         1.903         88         puopanizacial         3.170         3.474         3.500           27         propoxur         1.477         1.913         2.667         2.739         89         suifometuron         1.892         1.111         2.177         2.718           29         thieramulturon         1.633         2.067         2.439         90         terburturon         1.482         2.010         1.485         2.567         2.641         1.767           30         traidemethrin         5.000         5.050         4.982         2.173         91         traidemothrin         2.638         2.957         acalphose         2.674         2.641         1.767           31         aradiphosemethyl         3.168         2.175         3.230         2.318         2.000	22	metsulfuron	1.544	1.493	1.896	2.384	84	parathion	3.698	3.423	3.31	2.465
24         phoselone         4.25         3.923         4.122         2.209         86         pirimiphos-methyl         3.000         3.032         2.923         2.456           5         prochiraz         3.864         4.047         1.800         87         propachiror         1.822         2.244         2.13         4.407         1.803         2.957         3.70         3.474         3.250           27         propoxur         1.477         1.931         2.057         2.739         89         sulfometuron         1.832         2.171         2.171         2.718           28         terfacil         1.74         1.995         1.660         2.358         90         terbutryn         2.817         2.818         2.647         2.617         2.717           29         thifensulturon         1.653         1.267         2.718         92         antirolo         2.468         2.674         2.651         2.258         2.638         1.257           31         tridemorph         3.08         2.451         3.269         7         actiluorfen         2.053         2.258         2.638         1.267           32         alachiror         2.105         2.161         1.965 <td< td=""><td>23</td><td>parathion-methyl</td><td>2.373</td><td>2.333</td><td>2.211</td><td>2.061</td><td>85</td><td>phorate</td><td>3.000</td><td>2.905</td><td>2.365</td><td>1.110</td></td<>	23	parathion-methyl	2.373	2.333	2.211	2.061	85	phorate	3.000	2.905	2.365	1.110
25         prochoraz         3.864         3.645         4.047         1.850         87         propachin         1.832         2.244         2.173         2.214         2.270         1.903         88         propiconazole         2.957         3.170         3.474         3.250           27         propoxur         1.477         1.931         2.067         2.393         90         terburtyn         2.817         2.836         2.957         2.571         2.846         2.957         2.676         2.647         2.641         7.77         2.836         2.957         2.676         2.641         7.77         2.837         2.830         2.318         92         trichlorfon         1.462         2.010         1.453         2.646         2.707         94         acituorfen         2.462         2.574         2.641         7.76         3.249         2.246         2.707         94         acituorfen         2.053         2.292         2.536         1.257           33         amintrole         2.105         2.116         1.662         2.373         95         amentryn         2.477         2.227         1.85         1.597           34         aciphosentryl         3.163         2.236         2.608	24	phosalone	4.255	3.923	4.122	2.209	86	pirimiphos-methyl	3.000	3.032	2.923	2.456
26         propanil         2.173         2.214         2.870         1.903         88         propication         2.857         3.170         3.474         3.250           27         propoxur         1.474         1.995         1.660         2.369         90         terbutryn         2.817         2.836         2.957         2.676           29         thifensulfuron         1.653         1.636         2.093         3.378         91         thiral         0.531         0.846         0.984         5.250           30         trailomethrin         5.000         4.862         2.133         92         trichlorfor         1.462         2.010         1.452         2.474         3.474         1.66         2.077         94         acaligure         2.053         2.292         2.536         1.577           33         antirole         2.105         2.116         1.965         2.378         95         ametryn         2.474         3.428         2.453         1.453         5.1519           34         azinphos-metryl         3.164         2.373         95         ametryn         2.474         3.424         2.474         3.424         2.474         3.424         2.474         3.426         <	25	prochloraz	3.864	3.645	4.047	1.850	87	propachlor	1.832	2.244	2.135	4.060
27         propoxur         1.477         1.931         2.057         2.739         89         sulforeuron         1.892         1.711         2.177         2.716           28         terbacil         1.74         1.935         1.660         2.539         90         therbutyn         2.817         2.836         2.257         2.676           29         thifensulfuron         1.663         1.636         2.093         3.378         91         thiram         0.531         0.846         0.964         5.250           30         tridemorph         3.300         2.318         92         trichoton         1.462         2.010         1.453         2.641         1.767           32         alachior         2.079         2.581         2.646         2.707         94         acifluorien         2.435         1.551         1.575           34         azinphos-methyl         3.166         2.735         3.069         3.124         96         azinphos-ethyl         3.166         2.979         3.389         2.143           35         bernazore         1.531         1.375         1.389         2.262         97         bernavil         0.334         0.436         0.722         2.164	26	propanil	2.173	2.214	2.870	1.903	88	propiconazole	2.957	3.170	3.474	3.250
28         terbacil         1.7.4         1.995         1.660         2.359         90         terbutyn         2.817         2.836         2.979         2.673           30         trialomethrin         5.000         5.050         4.982         2.133         92         trichlorion         1.462         2.010         1.453         2.647           31         tridemorph         3.308         2.951         3.220         2.318         93         vinclozolin         2.426         2.574         2.641         1.757           32         alachlor         2.015         2.116         1.965         2.378         95         aaretyn         2.477         2.227         1.85         1.519           34         azinphos-methyl         3.166         2.373         3.069         3.124         96         azinphos-ethyl         3.166         2.979         3.389         2.143           35         bentazone         1.531         1.375         1.389         2.262         97         benomyl         3.243         0.436         0.332         2.474         3.244         2.453         2.455         2.253         2.455         2.253         2.455         2.53         2.455         2.53         2.455         <	27	propoxur	1.477	1.931	2.057	2.739	89	sulfometuron	1.892	1.711	2.177	2.718
29       thifensulturon       1.633       1.636       2.093       3.378       91       thiram       0.513       0.846       0.946       2.213         30       traiomethrin       5.000       5.050       4.982       2.133       92       trichlorfon       1.462       2.071       1.453       2.646         31       tridemorph       3.308       2.951       3.230       2.318       93       vinclozolin       2.426       2.574       2.661       1.575         32       alachior       2.079       2.581       2.646       2.707       94       actinutrin       2.477       2.227       1.85       1.519         34       azinphos-methyl       3.166       2.735       3.069       3.124       96       azinphos-ethyl       3.166       2.979       3.389       2.143         35       bentazone       1.531       1.375       1.389       2.262       97       beromofenoxin       0.343       0.436       0.732       2.196         36       bromoxynil       2.203       2.000       5.033       98       bromoxin       2.241       2.432       2.542       2.523       2.552       2.553       2.455         36       chloridzon	28	terbacil	1.74	1.995	1.660	2.359	90	terbutryn	2.817	2.836	2.957	2.676
30         traiomethrin         5.000         5.050         4.982         2.138         92         trichlorion         1.462         2.010         1.453         2.646         1.767           31         arditomorph         2.079         2.581         2.646         2.707         94         acifluorfen         2.053         2.292         2.536         1.257           33         amitrole         2.105         2.116         1.965         2.378         95         ametryn         2.477         2.227         1.85         1.519           34         azinphos-methyl         3.166         2.735         3.069         3.124         96         azinphos-rethyl         3.166         2.737         3.44         0.433         0.436         0.732         2.168           35         bentazone         1.531         1.375         1.389         2.262         97         beromotyni         0.334         0.436         0.732         2.168           36         chloridazon         2.037         1.428         1.459         100         carboxin         2.415         2.255         2.253         2.454           39         chloridazon         2.037         1.428         100         chloroburon         2.209 <td>29</td> <td>thifensulfuron</td> <td>1.653</td> <td>1.636</td> <td>2.093</td> <td>3.378</td> <td>91</td> <td>thiram</td> <td>0.531</td> <td>0.846</td> <td>0.984</td> <td>5.250</td>	29	thifensulfuron	1.653	1.636	2.093	3.378	91	thiram	0.531	0.846	0.984	5.250
31       tridemorph       3.308       2.951       3.230       2.318       93       windozclin       2.426       2.574       2.641       1.767         32       alachlor       2.015       2.116       1.965       2.378       95       ametryn       2.477       2.227       1.85       1.519         33       amitrole       2.105       2.116       1.965       2.378       95       ametryn       2.477       2.227       1.85       1.519         34       azinphos-metryl       3.166       2.735       3.069       3.124       96       azinphos-metryl       3.166       2.979       3.389       2.143         35       bernazone       1.531       1.375       1.389       2.262       97       bernompinos       0.334       0.436       0.732       2.196         37       carbendazim       2.110       1.911       1.740       3.127       99       carbaryl       2.093       2.083       1.908       2.873         38       chlorpopham       2.602       2.608       2.373       2.428       101       chlorotoluron       2.243       2.542       2.274       2.294         40       oycloate       2.633       2.362       2.41	30	tralomethrin	5.000	5.050	4.982	2.133	92	trichlorfon	1.462	2.010	1.453	2.647
32       alachlor       2.079       2.581       2.546       2.707       94       acliluoten       2.053       2.292       2.536       1.257         33       anilrole       2.105       2.116       1.965       2.116       1.965       3.166       2.979       3.389       2.143         34       azinphos-methyl       3.166       2.735       3.069       2.129       95       arenteryn       2.477       2.227       1.86       1.513         35       bentazone       1.531       1.375       1.389       2.262       97       benomyl       3.278       3.240       2.740       3.428         36       bromoxynil       2.230       2.336       2.000       5.033       98       bromotenxim       0.334       0.436       0.722       2.196         37       carbendazim       2.110       1.911       1.740       3.127       99       carbaryl       2.093       2.083       1.908       2.455         39       chloridazon       2.037       2.428       101       chlorotoluron       2.243       2.452       2.277       2.041       2.551         41       dichlobenil       2.326       2.481       1.907       102       oynanic	31	tridemorph	3.308	2.951	3.230	2.318	93	vinclozolin	2.426	2.574	2.641	1.767
33       amitrole       2.105       2.116       1.965       2.378       95       ametryn       2.477       2.227       1.85       1.519         34       azinphos-methyl       3.166       2.736       3.009       3.124       96       azinphos-enthyl       3.166       2.979       3.389       2.144         35       bentazone       1.531       1.375       1.389       2.262       97       benomolenoxim       0.334       0.436       0.732       2.196         36       bromoxynil       2.200       2.336       2.000       5.033       98       bromotenoxim       0.334       0.436       0.732       2.196         37       carbendazim       2.107       1.869       1.824       1.459       100       carboxin       2.415       2.255       2.233       2.455         39       chloridazon       2.037       1.869       1.824       1.459       100       carboxin       2.415       2.255       2.274       2.247       2.244         40       cyclotate       2.633       2.232       2.116       1.907       102       cyanazine       2.029       2.177       2.041       2.551         41       dichobenil       2.326       <	32	alachlor	2.079	2.581	2.646	2.707	94	acifluorfen	2.053	2.292	2.536	1.257
34       azinpnos-metnyi       3.166       2.73       3.069       3.124       96       azinpnos-etnyi       3.166       2.979       3.389       2.143         35       bentazone       1.531       1.375       1.389       2.262       97       benomyi       3.278       3.240       0.436       0.732       2.196         36       bromoxynil       2.230       2.336       2.000       5.033       98       bromotenoxim       0.334       0.436       0.732       2.196         37       carbendazim       2.110       1.911       1.740       3.127       99       carboxin       2.415       2.253       2.455         39       chlorpropham       2.602       2.608       2.373       2.428       101       chlorotoluron       2.443       2.542       2.274       2.244         40       cycloate       2.633       2.322       2.116       1.907       102       cyanzine       0.029       2.177       2.041       2.551         41       dichobenil       2.326       2.481       1.931       1.686       103       dicamba       0.301       0.416       0.321       2.171         4       diduat       6.000       5.757       5.5	33	amitrole	2.105	2.116	1.965	2.378	95	ametryn	2.477	2.227	1.85	1.519
35       bentazone       1.31       1.375       1.389       2.262       97       benomy       3.278       3.240       2.400       3.424       2.400       3.424       2.400       3.424       2.419       3.434       0.436       0.732       2.198         36       bromoxynil       2.301       1.911       1.740       3.127       99       carbaryl       2.093       2.083       1.908       2.837         37       carbendazim       2.101       1.911       1.740       3.127       99       carbaryl       2.093       2.043       2.243       2.542       2.274       2.944         39       chlorpropham       2.602       2.608       2.373       2.428       101       chlorotoluron       2.243       2.542       2.274       2.944         40       cycloate       2.633       2.232       2.116       1.907       102       cyanazire       2.009       2.117       2.041       2.551         41       dichubenil       2.326       2.481       1.931       1.686       103       dicarba       0.301       0.416       0.321       2.107         42       diflubenzuron       4.000       5.757       5.586       3.025       105	34	azinphos-methyl	3.166	2.735	3.069	3.124	96	azinphos-ethyl	3.166	2.979	3.389	2.143
36         bromoxyni         2.230         2.336         2.000         5.033         98         bromotenoxim         0.334         0.436         0.732         2.189           37         carbendazim         2.110         1.911         1.740         3.127         99         carboxin         2.415         2.255         2.253         2.455           38         chloridazon         2.037         1.869         1.824         1.457         100         carboxin         2.445         2.255         2.253         2.455           39         chloriopham         2.602         2.608         2.373         2.428         101         chloriopham         2.029         2.177         2.041         2.551           41         dichlobenil         2.326         2.481         1.931         1.666         103         dicamba         0.301         0.416         0.321         2.107           42         diflubenzuron         4.000         3.719         3.593         2.878         104         diclofop         4.204         3.708         3.918         3.745           44         endosulfan         4.000         4.018         3.626         1.389         107         ethalfluralin         3.602         3.179	35	bentazone	1.531	1.375	1.389	2.262	97	benomyl	3.278	3.240	2.740	3.428
37       carbendazim       2.110       1.911       1.740       3.127       99       carbaryl       2.093       2.083       1.908       2.837         38       chloridazon       2.037       1.869       1.824       1.459       100       carboxin       2.415       2.255       2.253       2.454         39       chlorpropham       2.602       2.608       2.373       2.428       101       chlorotoluron       2.243       2.542       2.274       2.294         40       oycloate       2.633       2.232       2.116       1.907       102       cyanazine       2.029       2.177       2.041       2.551         41       dichlobenil       2.326       2.481       1.931       1.686       103       dicamba       0.301       0.416       0.321       2.107         42       difubenzuron       4.000       3.719       3.539       2.878       104       diclohop       4.204       3.708       3.918       3.744         44       endosultan       4.093       4.138       4.008       3.549       106       DNOC       1.806       1.706       1.421       3.201       1.944         45       ethion       4.108       3.025	36	bromoxynil	2.230	2.336	2.000	5.033	98	bromotenoxim	0.334	0.436	0.732	2.196
33       chlordazon       2.037       1.869       1.824       1.439       1.00       catroxin       2.413       2.253       2.253       2.253       2.254       2.274       2.294         39       chlorpropham       2.602       2.608       2.373       2.428       101       chlorotoluron       2.243       2.542       2.274       2.294         41       dichobenil       2.326       2.481       1.931       1.686       103       dicamba       0.301       0.416       0.321       2.107         42       diflubenzuron       4.000       3.719       3.593       2.878       104       diclofop       4.204       3.708       3.918       3.745         43       diquat       6.000       5.757       5.586       3.025       105       diphenamid       2.079       2.111       2.44       1.645         44       endosulfan       4.093       4.138       4.008       3.549       106       DNOC       1.806       1.706       1.421       3.201       1.944         45       ethion       3.076       3.079       2.346       2.918       109       fenpropimorph       3.403       3.477       3.477       1.891         46	37	carbendazim	2.110	1.911	1.740	3.127	99	carbaryl	2.093	2.083	1.908	2.837
39         Chlopropham         2.602         2.608         2.373         2.428         101         Chlopropham         2.223         2.244         2.244         2.244         2.244         2.244         2.244         2.244         2.244         2.244         2.244         2.244         2.244         2.254           41         dichlobenil         2.326         2.481         1.907         102         cyanazine         2.029         2.177         2.041         2.551           42         diflubenzuron         4.000         3.719         3.593         2.878         104         diclofop         4.204         3.708         3.918         3.745           43         diquat         6.000         5.757         5.566         3.025         105         diphenamid         2.079         2.117         2.44         1.645           44         endosulfan         4.000         4.018         3.626         1.389         107         ethalfluratin         3.602         3.179         3.275         2.173           45         fenamiphos         2.426         2.587         2.445         4.187         108         etridiazole         3.000         3.132         3.021         1.984           47	38	chioridazon	2.037	1.869	1.824	1.459	100	carboxin	2.415	2.255	2.253	2.455
40       Gycloate       2.033       2.232       2.116       1.907       102       Cydnazine       2.029       2.177       2.041       2.501         41       dichlobenil       2.326       2.481       1.931       1.686       103       dicamba       0.301       0.416       0.321       2.107         42       diflubenzuron       4.000       3.719       3.593       2.878       104       diclofop       4.204       3.708       3.918       3.745         43       diquat       6.000       5.757       5.586       3.025       105       diphenamid       2.079       2.111       2.44       1.645         44       endosulfan       4.093       4.138       4.008       3.549       106       DNOC       1.806       1.766       1.421       3.201         45       ethion       4.000       4.018       3.626       1.389       107       ethalfluralin       3.602       3.179       3.275       2.177       2.184         46       fenamiphos       2.426       2.587       2.445       4.187       108       ethioralicale       3.000       3.132       3.021       1.984         47       fenthion       3.176       3.079	39	cniorpropnam	2.602	2.608	2.373	2.428	101	chiorotoluron	2.243	2.542	2.274	2.294
41       dichiobenii       2.32b       2.481       1.931       1.686       103       dicamba       0.301       0.416       0.321       2.107         42       diflubenzuron       4.000       3.719       3.593       2.878       104       diclofop       4.204       3.708       3.918       3.745         43       diquat       6.000       5.757       5.586       3.025       105       diphenamid       2.079       2.111       2.44       1.645         44       endosulfan       4.093       4.138       4.008       3.549       106       DNOC       1.806       1.706       1.421       3.201         45       ethion       4.000       4.018       3.626       1.389       107       ethalfluralin       3.602       3.179       3.275       2.173         46       fenamiphos       2.426       2.587       2.445       4.187       109       fentropionoph       3.403       3.477       3.471       1.894         48       glufosinate       2.000       2.049       1.899       2.913       110       fonofos       2.939       2.402       2.716       2.991         49       ioxynil       2.301       1.987       1.846	40	cycloate	2.633	2.232	2.116	1.907	102	cyanazine	2.029	2.177	2.041	2.551
42       difludenzuron       4.000       3.719       3.939       2.878       104       diclotop       4.204       3.708       3.918       3.745         43       diquat       6.000       5.757       5.586       3.025       105       diphenamid       2.079       2.111       2.44       1.645         44       endosulfan       4.093       4.138       4.008       3.626       1.389       107       ethalfluralin       3.602       3.179       3.275       2.173         46       fenamiphos       2.426       2.587       2.445       4.187       108       etridiazole       3.000       3.132       3.021       1.984         47       fenthion       3.176       3.079       2.346       2.918       109       fenpropimorph       3.403       3.477       3.477       1.891         48       glufosinate       2.000       2.049       1.899       2.913       110       fonofos       2.939       2.402       2.716       2.917         49       ioxynil       2.301       1.987       1.846       2.133       111       imazapyr       2.000       1.977       1.714       2.517         50       lindane       3.041       2.912<	41	dicniopenii	2.326	2.481	1.931	1.686	103	dicamba	0.301	0.416	0.321	2.107
43       diquat       6.000       5.757       5.586       3.025       105       dipnenamid       2.079       2.111       2.44       1.645         44       endosulfan       4.093       4.138       4.008       3.529       106       DNOC       1.806       1.706       1.421       3.201         45       ethion       4.000       4.018       3.626       1.389       107       ethalfluralin       3.602       3.179       3.275       2.173         46       fenamiphos       2.426       2.587       2.445       4.187       108       etridiazole       3.000       3.132       3.021       1.984         48       glufosinate       2.000       2.049       1.899       2.913       110       fonofos       2.939       2.402       2.716       2.991         49       ioxynil       2.301       1.987       1.846       2.133       111       imazapyr       2.000       1.977       1.714       2.517         50       lindane       3.041       2.912       3.031       2.779       112       isoporturon       2.029       2.066       2.07       2.803         51       methabenzthiazuron       2.722       2.252       2.064	42	diflubenzuron	4.000	3.719	3.593	2.878	104	diclotop	4.204	3.708	3.918	3.745
44       effodSultarin       4.093       4.138       4.008       3.349       106       DNOC       1.806       1.706       1.421       3.201         45       ethion       4.000       4.018       3.626       1.389       107       ethalfluralin       3.602       3.179       3.275       2.173         46       fenamiphos       2.426       2.587       2.445       4.187       108       etridiazole       3.000       3.132       3.021       1.984         47       fenthion       3.176       3.079       2.346       2.918       109       fenpropimorph       3.403       3.477       3.477       1.894         48       glufosinate       2.000       2.049       1.899       2.913       110       fonofos       2.939       2.402       2.716       2.991         49       ioxynil       2.301       1.987       1.846       2.133       111       imazapyr       2.000       1.977       1.714       2.517         50       lindane       3.041       2.912       3.031       2.779       112       isoproturon       2.029       2.086       2.07       2.803         51       methosychlor       4.903       4.766       2.242 </td <td>43</td> <td>diquat</td> <td>6.000</td> <td>5./5/</td> <td>5.586</td> <td>3.025</td> <td>105</td> <td>aipnenamia</td> <td>2.079</td> <td>2.111</td> <td>2.44</td> <td>1.645</td>	43	diquat	6.000	5./5/	5.586	3.025	105	aipnenamia	2.079	2.111	2.44	1.645
43       ethioli       4.000       4.018       5.020       1.389       107       ethialutatiin       5.802       5.179       5.275       2.173         46       fenamiphos       2.426       2.587       2.445       4.187       108       etridiazole       3.000       3.132       3.021       1.984         47       fenthion       3.176       3.079       2.346       2.918       109       fenzopimph       3.403       3.477       3.477       1.891         48       glufosinate       2.000       2.049       1.892       2.913       110       fonofos       2.939       2.402       2.716       2.991         49       ioxynil       2.301       1.987       1.846       2.133       111       imazapyr       2.000       1.977       1.714       2.517         50       lindane       3.041       2.912       3.031       2.779       112       isoproturon       2.029       2.086       2.07       2.803         51       methabenzthiazuron       2.722       2.252       2.064       2.895       113       mecoprop       2.103       2.281       2.06       1.000         52       methoxychlor       4.903       4.766       4	44	endosulian	4.093	4.130	4.008	3.549	100	DINOC	1.600	1.700	1.421	3.201
46       Initiality index       2.420       2.567       2.4445       4.167       106       fendrolative       3.000       3.132       3.132       3.132       3.132       3.132       3.132       3.132       3.132       3.132       3.132       3.132       3.137       3.477       1.891         47       fenthion       3.176       3.079       2.346       2.918       109       fenpropimorph       3.403       3.477       3.477       1.891         48       glufosinate       2.000       2.049       1.899       2.913       110       fonofos       2.939       2.402       2.716       2.991         50       lindane       3.041       2.912       3.031       2.779       112       isoproturon       2.029       2.086       2.07       2.803         51       methabenzthiazuron       2.722       2.252       2.064       2.895       113       mecoprop       2.103       2.281       2.06       1.000         52       methoxychlor       4.903       4.766       4.26       2.412       114       methomyl       1.857       2.084       1.862       3.428         53       napropamide       2.845       3.023       2.866       5.644	40	fonominhoo	4.000	4.010	3.020 0.445	1.309	107	etridiozolo	3.002	0.179	3.275	2.173
47       Interflution       5.176       5.079       2.346       2.916       109       Interplupininupin       5.403       3.477       3.477       1.917         48       glufosinate       2.000       2.049       1.899       2.913       110       fonofos       2.939       2.402       2.716       2.991         49       ioxynil       2.301       1.987       1.846       2.133       111       imazapyr       2.000       1.977       1.714       2.517         50       lindane       3.041       2.912       3.031       2.779       112       isoproturon       2.029       2.086       2.07       2.803         51       methabenzthiazuron       2.722       2.252       2.064       2.895       113       mecoprop       2.103       2.281       2.06       1.000         52       methoxychlor       4.903       4.766       4.26       2.412       114       methomyl       1.857       2.084       1.862       3.428         53       napropamide       2.845       3.023       2.866       5.644       115       molinate       2.278       1.993       1.764       3.672         54       permethrin       5.000       4.442	40	fonthion	2.420	2.007	2.440	4.107	100	forpronimorph	3.000	0.102 0.477	3.021	1.904
43glubsinate2.0002.0491.0592.913110futbols2.9392.4022.7102.99149ioxynil2.3011.9871.8462.133111imazapyr2.0001.9771.7142.51750lindane3.0412.9123.0312.779112isoproturon2.0292.0862.072.80351methabenzthiazuron2.7222.2522.0642.895113mecoprop2.1032.2812.061.00052methoxychlor4.9034.7664.262.412114methomyl1.8572.0841.8623.42853napropamide2.8453.0232.8665.644115molinate2.2781.9931.7643.67254permethrin5.0004.4424.2383.909116pebulate3.1552.3422.8241.00055pirimicarb2.8692.5372.8194.117117picloram1.2041.6071.2651.41956prometryn2.4112.1992.2662.462118prometon3.1762.7913.0123.44757propham1.2721.2141.5351.564119propazine2.1872.4532.6093.21558simazine2.0612.4082.1902.212120propyzamide2.4032.5132.7451.73159terbuthylazine2.485	47 70	dufocipato	3.170	3.079	2.340	2.910	109	fonofoc	2 020	0.477 0.400	0.477	2 001
49       ItoXyIII       2.301       1.967       1.046       2.153       111       Ititazapyi       2.000       1.977       1.714       2.317         50       lindane       3.041       2.912       3.031       2.779       112       isoproturon       2.029       2.086       2.07       2.803         51       methabenzthiazuron       2.722       2.252       2.064       2.895       113       mecoprop       2.103       2.281       2.06       1.000         52       methoxychlor       4.903       4.766       4.26       2.412       114       methomyl       1.857       2.084       1.862       3.428         53       napropamide       2.845       3.023       2.866       5.644       115       molinate       2.278       1.993       1.764       3.672         54       permethrin       5.000       4.442       4.238       3.909       116       pebulate       3.155       2.342       2.824       1.000         55       pirimicarb       2.869       2.537       2.819       4.117       117       picloram       1.204       1.607       1.265       1.419         56       prometryn       2.411       2.192       2.26	40	giulosinale	2.000	2.049	1.099	2.910	110	imozonyr	2.939	2.402	2.710	2.991
50       1112       151       112       151       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       112       150       113       mecoprop       2.103       2.281       2.060       1.000	49 50	lindane	2.301	2 012	3 031	2.133	112	isoproturon	2.000	2 086	2.07	2.017
51       methoxychlor       2.722       2.202       2.004       2.895       113       metophop       2.103       2.201       2.004       1.000         52       methoxychlor       4.903       4.766       4.26       2.412       114       methomyl       1.857       2.084       1.862       3.428         53       napropamide       2.845       3.023       2.866       5.644       115       molinate       2.278       1.993       1.764       3.672         54       permethrin       5.000       4.442       4.238       3.909       116       pebulate       3.155       2.342       2.844       1.000         55       pirimicarb       2.869       2.537       2.819       4.117       117       picloram       1.204       1.607       1.265       1.419         56       prometryn       2.411       2.190       2.266       2.462       118       prometon       3.176       2.791       3.012       3.447         57       propham       1.272       1.214       1.535       1.564       119       propazine       2.187       2.453       2.609       3.215         58       simazine       2.061       2.408       2.190	50	mothohonzthiazuron	0.041	2.912	2.051	2.119	112	moconron	2.029	2.000	2.07	2.003
52       Interforycrifor       4.303       4.703       4.203       2.412       114       Interform       1.037       2.004       1.062       3.420         53       napropamide       2.845       3.023       2.866       5.644       115       molinate       2.278       1.993       1.764       3.672         54       permethrin       5.000       4.442       4.238       3.909       116       pebulate       3.155       2.342       2.844       1.000         55       pirimicarb       2.869       2.537       2.819       4.117       117       picloram       1.204       1.607       1.265       1.419         56       prometryn       2.411       2.199       2.266       2.462       118       prometon       3.176       2.791       3.012       3.447         57       propham       1.272       1.214       1.535       1.564       119       propazine       2.187       2.453       2.609       3.215         58       simazine       2.061       2.408       2.190       2.212       120       propyzamide       2.403       2.513       2.745       1.731         59       terbuthylazine       2.485       2.683       2.	52	methoxychlor	2.722	1 766	2.004	2.090	11/	methomyl	2.103	2.201	2.00	3 428
53Informative2.6436.6232.6006.644113Informative2.2701.3531.7643.07254permethrin5.0004.4424.2383.909116pebulate3.1552.3422.8241.00055pirimicarb2.8692.5372.8194.117117picloram1.2041.6071.2651.41956prometryn2.4112.1992.2662.462118prometon3.1762.7913.0123.44757propham1.2721.2141.5351.564119propazine2.1872.4532.6093.21558simazine2.0612.4082.1902.212120propyzamide2.4032.5132.7451.73159terbuthylazine2.4852.6832.9202.352121terbufos2.6982.6663.1174.15560thiodicarb2.5442.9412.8923.439122thiobencarb2.9542.5042.4643.98661triallate3.2683.2933.9333.917123triadimenol2.3572.5272.9692.67762vernolate2.4152.2772.3304.429124trifluralin3.8073.5462.8212.461	52	napropamide	2.845	3 023	2,866	5.614	115	molinato	2 278	1 003	1.002	3 672
54perinternin5.0004.4424.2005.505110perutate5.1052.0522.0241.00055pirimicarb2.8692.5372.8194.117117picloram1.2041.6071.2651.41956prometryn2.4112.1992.2662.462118prometon3.1762.7913.0123.44757propham1.2721.2141.5351.564119propazine2.1872.4532.6093.21558simazine2.0612.4082.1902.212120propyzamide2.4032.5132.7451.73159terbuthylazine2.4852.6832.9202.352121terbufos2.6982.6663.1174.15560thiodicarb2.5442.9412.8923.439122thiobencarb2.9542.5042.4643.98661triallate3.2683.2933.9333.917123triadimenol2.3572.5272.9692.67762vernolate2.4152.2772.3304.429124trifluralin3.8073.5462.8212.461	5/	nermethrin	5.040	1 112	1 238	3 000	116	nebulate	2.270	0.340	2 824	1 000
56prometryn2.4112.1992.2662.462118prometon3.1762.7913.0123.44757propham1.2721.2141.5351.564119propazine2.1872.4532.6093.21558simazine2.0612.4082.1902.212120propyzamide2.4032.5132.7451.73159terbuthylazine2.4852.6832.9202.352121terbufos2.6982.6663.1174.15560thiodicarb2.5442.9412.8923.439122thiobencarb2.9542.5042.4643.98661triallate3.2683.2933.9333.917123triadimenol2.3572.5272.9692.67762vernolate2.4152.2772.3304.429124trifluralin3.8073.5462.8212.461	55	nirimicarh	2 860	7.742 2.527	2 810	0.909 117	117	pedulate	1 20/	2.042	1 265	1 / 10
57propham1.2721.2141.5351.564119propazine2.1872.4532.6093.21558simazine2.0612.4082.1902.212120propyzamide2.4032.5132.7451.73159terbuthylazine2.4852.6832.9202.352121terbufos2.6982.6663.1174.15560thiodicarb2.5442.9412.8923.439122thiobencarb2.9542.5042.4643.98661triallate3.2683.2933.9333.917123triadimenol2.3572.5272.9692.67762vernolate2.4152.2772.3304.429124trifluralin3.8073.5462.8212.461	56	prometrue	2.003	2.007	2.019	2/162	112	promoton	2 176	2 701	3 012	3 1/17
57propriati1.2121.2141.0001.004119propriati2.1072.4032.0053.21558simazine2.0612.4082.1902.212120propyzamide2.4032.5132.7451.73159terbuthylazine2.4852.6832.9202.352121terbufos2.6982.6663.1174.15560thiodicarb2.5442.9412.8923.439122thiobencarb2.9542.5042.4643.98661triallate3.2683.2933.9333.917123triadimenol2.3572.5272.9692.67762vernolate2.4152.2772.3304.429124trifluralin3.8073.5462.8212.461	57	nronham	1 979	1 214	1 525	1 564	110	nronazina	2 187	2453	2 600	3 215
Solution         2.405         2.405         2.105         2.112         120         propyzanide         2.405         2.113         2.143         1.131           59         terbuthylazine         2.485         2.683         2.920         2.352         121         terbufos         2.698         2.666         3.117         4.155           60         thiodicarb         2.544         2.941         2.892         3.439         122         thiobencarb         2.954         2.504         2.464         3.986           61         triallate         3.268         3.293         3.933         3.917         123         triadimenol         2.357         2.527         2.969         2.677           62         vernolate         2.415         2.277         2.330         4.429         124         trifluralin         3.807         3.546         2.821         2.461	58	simazina	2 061	2 408	2 100	2 212	120	nronyzamida	2 403	2 512	2 745	1 721
60         thiodicarb         2.544         2.941         2.892         3.439         122         thiobencarb         2.954         2.504         2.464         3.986           61         triallate         3.268         3.293         3.933         3.917         123         triadimenol         2.357         2.527         2.969         2.677           62         vernolate         2.415         2.277         2.330         4.429         124         trifluralin         3.807         3.546         2.821         2.461	59	terhuthvlazine	2 485	2 683	2,920	2 352	121	terhulos	2 698	2.515	3 117	4 155
61         triallate         3.268         3.293         3.933         3.917         123         triadimenol         2.357         2.527         2.969         2.677           62         vernolate         2.415         2.277         2.330         4.429         124         trifluralin         3.807         3.546         2.821         2.461	60	thiodicarh	2 544	2 941	2 892	3 439	122	thiohencarh	2 954	2 504	2 464	3 986
62         vernolate         2.415         2.277         2.330         4.429         124         trifluralin         3.807         3.546         2.821         2.461	61	triallate	3,268	3,293	3,933	3,917	123	triadimenol	2.357	2.527	2,969	2 677
	62	vernolate	2.415	2.277	2.330	4.429	124	trifluralin	3.807	3.546	2.821	2.461

<sup>*a*</sup> Training set, molecules 1–62; validation set, molecules 63–93; test set, molecules 94–124.

and  $q^{ik}$  represent the  $j^{th}$  and  $k^{th}$  coordinates (j, k = x, y, z) of the *i*th atom, respectively, and  $\overline{q}$  is the corresponding average value. The last descriptor that appeared in the model is highest eigenvalue n.2 Burden matrix/weighted

by atomic masses (BEHm2). BCUT descriptors are defined as eigenvalues of a modified connectivity matrix, which could be called Burden matrix B. The B matrix is defined as follows: The diagonal elements  $B_{ii}$  are the atomic

#### Table 2. Descriptors Used in Model Construction

no.	symbol	class	meaning
1	HTp	GETAWAY	H total index/weigthed by atomic polarizabilities
2	MATS6e	2D autocorrelation	Moran autocorrelation lag-6/ weighted by atomic Sanderson electronegativities
3	G3v	WHIM	third-component symmetry directional WHIM index/weighted by atomic van der Waals volumes
4	Mor05m	3D-MoRSE	3D-MoRSE-signal05/weighted by atomic masses
5	G1m	WHIM	first-component symmetry directional WHIM index/weighted by atomic masses
6	MATS4p	2D autocorrelation	Moran autocorrelation lag-4/weighted by atomic polarizabilities
7	BEHm2	BCUT	highest eigenvalue n.2 Burden matrix/weighted by atomic masses

 Table 3. Correlation Matrix for the Seven Selected Descriptors

	НТр	MATS6e	G3v	Mor05m	G1m	MATS4p	BEHm2
HTp	1						
MATS6e	0.0337	1					
G3v	0.209	0.001	1				
Mor05m	0.0056	0.0134	0.0072	1			
G1m	0.0575	0.0021	0.1073	0.0005	1		
MATS4p	0.0202	0.0001	0.0001	0.0331	0.0386	1	
BEHm2	0.1867	0.3702	0.0035	0.02	0.0004	0.0297	1

number  $Z_i$  of the atoms; the off-diagonal elements  $B_{ij}$  representing two bonded atoms *i* and *j* are equal to  $\pi^* \times 10^{-1}$ , where  $\pi^*$  is conventional bond order, that is, 0.1, 0.2, 0.3, and 0.15 for single, double, triple, and aromatic bonds, respectively; off-diagonal elements  $B_{ij}$  corresponding to terminal bonds are augmented by 0.01; all other matrix elements are set to 0.001 (29).

### **RESULTS AND DISCUSSION**

The prediction ability of QSAR/QSPR models is affected by two factors. One is the descriptors, which should carry enough information of molecular structure for the interpretation of the activity/property. The other is the modeling method employed (*30*). The number of descriptors available for QSAR/ QSPR studies is often so large that it is difficult to obtain a model including all of them. Therefore, identifying important descriptors certainly plays an important role in QSAR/QSPR. Descriptors should represent the maximum information in activity variations, and collinearity among them must be kept to a minimum.

The seven descriptors that have been selected using SPA are shown in **Table 2**. As can be seen from the correlation matrix (**Table 3**), there is no significant correlation between the selected descriptors. These descriptors were used for both linear and nonlinear models.

To build and test the models, the data set comprising 124 compounds was separated into a training set of 62 compounds, a validation set of 31 compounds, and a test set of 31 compounds. By using the training set, with the seven selected descriptors, the following linear model was obtained:

Log  $K_{OC} = 1.72965 + 0.333407HTp + 0.936504MATS6e$ + 0.78916G3v + 0.122569Mor05m + 4.201647G1m + 1.210337MATS4p - 0.711055BEHm2

This model was then used to predict the validation and test data. The prediction results are given in **Table 1**.

To construct an ANN model, a three-layer network with a sigmoid transfer function was employed. Before the networks were trained, the input values were normalized between -1 and 1. The initial weights were selected randomly between -0.3 and 0.3. The number of nodes in the hidden layer, as well as the learning rates and momentum values, were optimized. For this purpose,

 Table 4. Architecture and Training Settings for the ANN Models

<u> </u>	
no. of nodes in the input layer	$\frac{7+1^{a}}{6}$
no. of nodes in the output layer	1
earning rate	0.376
nomentum	0.628
no. of iterations	10
ransfer function	sigmoid

<sup>a</sup> Bias.



Figure 1. Plot of calculated soil sorption coefficients (log  $K_{OC}$ ) against experimental values.

the network was trained with different numbers of nodes in the hidden layer, and the root-mean-square error (RMSE) between network outputs and target values was employed as performance metric. **Table 4** shows the architecture and training settings of the optimized network.

It should be noted that the training of the network for the prediction of log  $K_{OC}$  was interrupted when the RMSE of the validation set started to increase, to avoid overfitting. To select the best weight update function, two statistical methods were considered for evaluating the resulting models, namely, leave-one-out cross-validation (Q<sup>2</sup> LOO) and prediction standard error of estimation (SEP).

The compounds in the test set were not used during the training process and were reserved to evaluate the predictive power of the generated ANN. The ANN-calculated values of log  $K_{OC}$  for training, validation, and test sets are shown in **Table 1**. Figure 1 shows the experimental values versus the predicted values by SPA-ANN. The residuals of the ANN calculated values of log  $K_{OC}$  are plotted against the experimental values in Figure 2. The presence of residuals at both sides of the zero line indicates that no systematic error exists in the development of the ANN model. For comparison, we also calculated  $K_{OC}$  by using the EPI package as shown in **Table 1**.

For evaluation of the predictive ability of the models, we employed the determination coefficient ( $R^2$ ), root-mean-square error of prediction (RMSEP), relative standard error of prediction



**Figure 2.** Plot of residuals versus experimental values of soil sorption coefficients (log  $K_{OC}$ ).

Table	5.	Comparison	of	the	Statistical	Parameters	Obtained	Using	the
SPA-N	1LR	and SPA-AN	IN I	Node	els				

para	meters	SPA-ANN	SPA-MLR	EPI
	training set	0.2824	0.4202	
RMSEP	validation set	0.3007	0.3992	1.3200
	test set	0.2888	0.3705	
	training set	9.8423	14.646	
RSEP (%)	validation set	11.377	15.102	48.085
	test set	11.164	14.324	
	training set	6.0120	7.4011	
MAE (%)	validation set	8.8812	10.149	9.0304
. ,	test set	8.5345	9.7164	
	training set	0.9314	0.8402	
R <sup>2</sup>	validation set	0.9196	0.8262	0.0052
	test set	0.9029	0.8199	
	training set	814.57	315.50	
F statistical	validation set	331.49	137.85	0.6333
	test set	269.77	132.05	
	training set	28.541	17.762	
t test	validation set	18.207	11741	0.7958
	test set	16.425	11.491	

(RSEP), and mean absolute error (MAE) values (31), which are defined as

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{\text{pred}} - y_{\text{obs}})^{2}}{\sum_{i=1}^{n} (y_{\text{obs}} - y_{\text{meas}})^{2}}$$
$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n} (y_{\text{pred}} - y_{\text{obs}})^{2}}{n}}$$

RSEP (%) = 100 × 
$$\sqrt{\frac{\sum_{i=1}^{n} (y_{\text{pred}} - y_{\text{obs}})^2}{\sum_{i=1}^{n} (y_{\text{obs}})^2}}$$

MAE (%) = 
$$\frac{100}{n} \times \sqrt{\sum_{i=1}^{n} |(y_{\text{pred}} - y_{\text{obs}})|}$$

where  $y_{\text{pred}}$  is the predicted value of the property under consideration,  $y_{\text{obs}}$  is the experimental value, and *n* is the number of samples in the set. These statistical parameters for SPA-MLR, SPA-ANN, and EPI are shown in **Table 5**. As can be seen, SPA-ANN provided the most accurate predictions of log  $K_{\text{OC}}$  for the pesticides employed in the study.

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