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Quantitative Structure-property Relationship Model Based on Artificial Neural Network

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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ABSTRACT

Artificial neural network (ANN) has been widely researched and applied in chemical process, because of its parallel processing and excellent nonlinear mapping ability, with strong robustness and fault tolerance. By using artificial neural network to establish the model between the properties of mixture and its molecular structure, more accurate data can be predicted and obtained than those determined by experiment. This paper summarizes the development process of artificial neural network and analyzes the application of ANN in quantitative structure-property relationship model (QSPR). It is pointed out that QSPR model combined with artificial neural network can effectively predict the properties of compounds or mixtures, which can shorten the experimental testing process and is able to be widely used with less limitation. It has important significance in application of new biomass fuel, the analysis of the pollution, prediction of the risk of dangerous chemical properties and so on. In the future, there will be broader application space of ANN-QSPR model.

Keywords: Artificial neural network; quantitative structure-property relationship; property estimation; RBF neural network; BP network.

1. INTRODUCTION

Quantitative structure-property relationship model is a property estimation method, the basic idea of which is that changes in molecular structure can reflect the changes in physical and chemical properties [1]. It is widely used in petroleum product development, ionic liquid

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research, drug design, and toxicity analysis of mixed pollutants [2-6]. QSPR model is based on chemical structure rather than experimental data to extract chemical information and it can be established without other empirical parameters, which makes it have a wide range of application and good prediction ability. What's more, the traditional study of QSPR focuses on the relationship between structure and properties of single component compounds, but in practice we often encounter the problem of dealing with multi-component mixtures. Compared with pure substance QSPR research, the properties of mixtures are determined by not only the structure of components in mixtures, but also the content of each component and the interaction between components, which has many influencing factors and more complex relationship [7].

Artificial neural network (ANN), an important module in the field of artificial intelligence, provides powerful technical support for the research of QSPR model of both pure compounds and mixture, due to its significant advantage such as parallel processing, distributed storage and fault tolerance, self-learning, self-organization and self-adaptation [8,9]. The QSPR model based on artificial neural network is simple to use and has high prediction accuracy. It has significant advantages compared with the traditional empirical model and the group contribution method. Traditional empirical model has complex process and complicated steps, which takes a great deal of manpower and resources. While, the group contribution method has the disadvantage that it cannot show the influence of the surrounding environment on molecules [1,10].

In this paper the development and the applied methods of artificial neural network is summarized, and the research progress of artificial neural network in quantitative structure-property relationship model is reviewed.

2. ARTIFICIAL NEURAL NETWORK AND THE OPERATING PRINCIPLE

2.1 The Development History and Characteristics of Neural Network

The establishment of artificial neural networks is based on the abstraction of human brain, imitating the structure and function of human brain to form different network according to different connection modes with strong information processing ability, which can be applied to deal with practical problems of multiple nodes and multiple output points [11].

The research on Artificial Neural Network (ANN) began in the 1940s. In 1943, psychologist McCulloch and mathematical scientist Pitts [12], first proposed a simple Neural Networks model. The input and output are both binary numbers, and the input has fixed weights. Some logical relationships can be realized by using this simple network, which started the exploration of artificial neural network. In 1949, Hebb [13] first proposed a rule to adjust the connection weights of neural networks, which is usually called Hebb learning rule. The basic idea is that when two neurons are excited at the same time, their connection strength increases. In 1969, M. Minsky [14] pointed out that the function of simple linear perceptron is limited, and it cannot solve the classification problem of two kinds of linearly indivisible samples. To solve this problem, hidden layer nodes must be added. But for multi-layer networks, how to find an effective learning algorithm is still a difficult problem to solve, so it put neural network research at a low ebb throughout the 1970s. By 1982, physicist Hopfield [15,16] published two articles on neural networks which aroused great repercussions. He proposed a feedback interconnection network and defined an energy function as a function of the state and connection weights of neurons, which could be used to solve associative memory and optimization problems, providing theoretical guidance for the construction and learning of artificial neural network. In 1986, Werbos et al. [17] analyzed and optimized the multi-layer back propagation algorithm with nonlinear continuous transfer function, namely BP algorithm, and proposed an effective algorithm for weight adjustment for the first time. In 2006, Hinton et al. [18] pointed out that high-dimensional data can be converted to low-dimensional codes by training a multilayer neural network with a small central layer to reconstruct high-dimensional input vectors and proposed an effective way of initializing the weights that allows deep autoencoder networks to learn low-dimensional codes, which brought the concept of "deep learning" to neural network researchers for the first time, which has been rapidly developed since then.

With the development of computer hardware and neural network theory, ANN has been widely applied to many fields, such as process optimization and control [19-23], automatic control and forecasting of power systems [24,25], medicine [26,27], intelligent driving [28-30], fault

diagnosis [31-33], image recognition [34-36] signal Processing [37], exergy efficiency and so on. Artificial neural network provides a new method for the problems that are difficult to solve by traditional technologies, improves research efficiency, which is beneficial to the development of various fields.

There are various neural network models using different algorithms: back propagation neural network (BP), radial basis function neural network (RBFNN), self-organizing feature mapping network (SOM), counter propagation neural network (CPNN) and wavelet neural network (WNN), etc [38-40]. Among them, RBFNN and BP network is more and more widely used in chemical progress because of their simple optimization process and strong nonlinear fitting ability. This paper will briefly introduce the operating principle of BP network and RBFNN, which are usually applied in establishing quantitative structure-property relationship model.

2.2 BP Neural Network

Error-back Propagation Network, abbreviated as BP neural network, is the most widely used neural network model in chemical research. BP network is a multi-layer forward network, which is divided into input layer, hidden layer and output layer. All layers are interconnected and there is no mutual connection between neurons in the same layer. The basic processing unit of BP network is nonlinear input-output relationship. Its structure is shown in Fig. 1.

X_P、Y_P represent the input signal and the output signal, i、j、k represent the number of layer, W_{ij} and V_{kj} represent the weight of each layer.

The standard BP neural network usually selects Sigmoid function as the activation function to simulate the characteristics of neurons.

$$f(x) = \frac{1}{1 + e^{-x}}\# \qquad (1)$$

The learning process of BP algorithm consists of forward propagation and back propagation. In the process of forward propagation, the information enters the network from the input layer, and then processed by the hidden layer and transmitted to the output layer to obtain the predicted value, which is compared with the target value. The state of neurons in each layer only affects the state of the next layer. If the desired output cannot be obtained in the output layer, it will turn to back propagation and return the error signal along the original connection path. By modifying the connection weight between neurons in each layer, the error signal will be minimized.

2.3 RBF Neural Network

Radial basis function neural network (RBFNN) is also a commonly used neural network model, which has the advantages of good approximation, simple optimization process and fast training speed. It has been widely used in QSPR research [41,42].

Similar to BP network, RBFNN is also a forward layered neural network, and its structure can be described by a three-layer network, as shown in Fig. 1. The first layer is the input layer, which usually inputs the structural parameters of molecules, the second layer is the hidden layer, that is, the radial basis function layer, and the third layer is the output layer. The input layer only inputs information without other processing. The hidden layer is usually composed of a series of RBF functions, which usually include Gaussian function, spline function and quadratic function. The most commonly used RBF function is Gaussian function

$$h_j(x) = exp\left(-||x - c_j||^2 / r_j^2\right)\# \qquad (2)$$

x is the input vector, j represents the number RBF function, $h_j(x)$ is the output of the RBF function, c_j is the center of the hidden layer node, and r_j is the radius of the RBF.

The main difference between the two is that BP network takes the inner product of weight and input as the net input of the network, while RBF network takes the Euclidean distance between the input vector of training samples and the weight vector of hidden layer nodes as the net input. Theoretically, RBFNN can approximate any continuous nonlinear function like BP network. When BP network is used for function approximation, the weight is adjusted by gradient descent method. This method has some disadvantages, such as slow convergence speed and local minimum, so there are certain application limitations. RBFNN is superior to BP network in this respect. Its best approximation ability makes it have good application value.

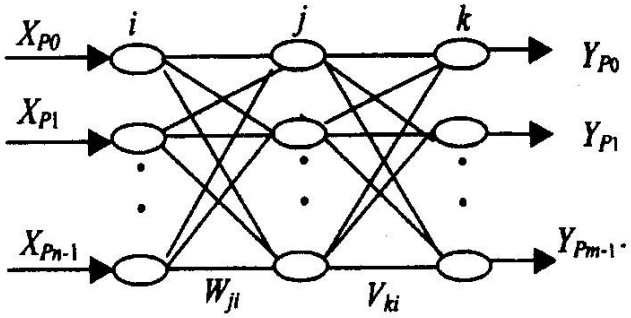

Fig. 1. The basic structure of artificial neural network

3. ESTABLISHMENT OF QSPR MODEL WITH ARTIFICIAL NEURAL NETWORK

The prediction of novel fuel properties is an important application field of ANN-QSPR model. It has been a research hotspot in the fuel field to use advanced chemical and biological technology to research new alternative fuels to replace the diesel and gasoline fuels which will be exhausted, while reducing production costs and improving process output.

Kessler et al. [43] established an artificial neural network analyzing quantitative structure-property relationships model to predict the cetane number of furans and their derivatives in biofuels. Cetane number (CN) is one of the most important parameters for evaluating a fuel for use in a diesel engine, a measure of the fuel's ignition quality. Ignition Quality Tester (IQT) is the traditional methods to determine CN. The measurement instrument is a four-stroke single cylinder indirect injection diesel engine that can change the compression ratio continuously. The cetane number was determined by comparing the ignition performance of the sample with the standard fuel. This is done by changing the compression ratio, or handwheel reading, of each sample under standard operating conditions and of two engines with standard fuels that include the sample in the middle and have cetane values that differ by no more than 5.5. The cetane number was then calculated by interpolation. But this determination method is complex with large raw material consumption and long determination period, the sheer number of potential fuel molecules makes testing prohibitive in terms of both cost and time.

Kessler adopts BP network approach since it relatively more robust across multiple molecular classes/families due to its nonlinear architecture, which allows for a representation of very complex relationships between input and output vectors in prediction of CN. The cetane number data used for the core data set was obtained from sets found in the NREL Compendium of Experimental Cetane Number Data [44] and other sources [45,46]. It contains 284 compounds in total. By the analysis of compound structures using MarvinSketch (ChemAxon Ltd.) [47] and the NCI online calculator [48], 1667 QSPR molecular descriptors was obtained, which was reduced to 15 to short the build-time of the artificial network networks and obtain better prediction accuracy in the following progress. The 15 QSPR molecular descriptors was selected to be the most influential descriptors in regards to CN prediction for this database using an iterative regression analysis technique, which is shown in Table 1.

They build an artificial neural network prediction model based on trial and error experiment. The basic structure of this network includes the 15 molecular descriptors as input data, two hidden layers of 32 neurons each, and a single output (CN). Two hidden layers, rather than one, are used in order to capture the highly nonlinear relationship between QSPR descriptors and CN. For network learning, the Levenberg-Marquardt backpropagation involving stochastic gradient descent was chosen as the learning method of this network. The optimization function used for the regression was the mean squared error function, where the network converges to the point of least error relative to the core data set as a whole.

The database is divided into three parts for network learning, validation and testing, accounting for 65%, 25% and 10% respectively. ANN is trained according to the data set and adjusts network parameters according to the RMSE value between the predicted value and

Table 1. Glossary of descriptor terminology [43]

Descriptor	Definition
Mor32e	3D MoRSE - Signal 32/Weighted by Sanderson electronegativity
ESpm05u	Spectral moment of order 2 from edge adjacency mat.
CIC1	Complementary Information Content Index (neighborhood symmetry of 1-order)
RDF035u	Radial Distribution Function - 035/unweighted
nROR	Number of ethers
nROH	Number of hydroxyl groups
L/Bw	Length-to-breadth ratio by WHIM
RDF090m	Radial Distribution Function - 090/weighted by mass
nHDon	Number of donor atoms for H-bonds (N and O)
RDF020p	Radial Distribution Function - 020/weighted by polarizability
nOHp	Number of primary alcohols
EEig08x	Eigenvalue n. 8 from augmented edge adjacency mat. weighted by bond order
O-059	Al-O-Al/Atom-centered fragments
G3s	3rd component symmetry direction WHIM index/weighted by I-state
GATS8m	Geary autocorrelation of lag 8 weighted by mass

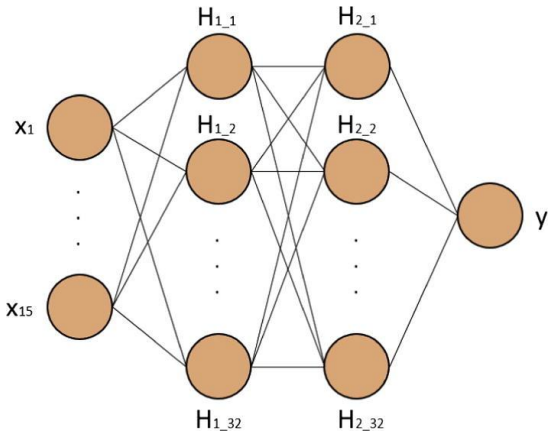

Fig. 2. Model architecture including inputs, two hidden layers of 32 neurons, and an output [43]

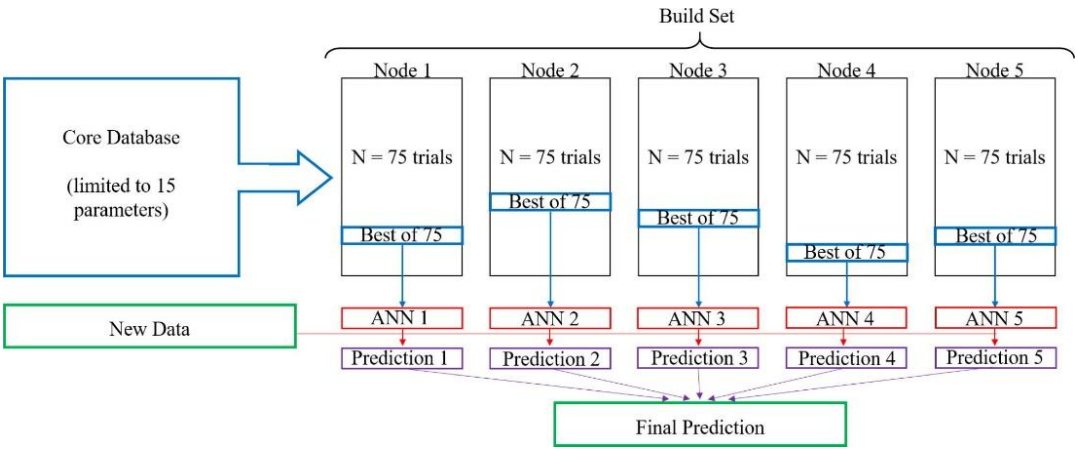

Fig. 3. Simulation diagram of the build set construction procedure [43]

the experimental value,until there was no significant improvement in the performance of the validation proportion. Finally, five optimal ANN structures are selected. By averaging the predicted values of the five networks, the result is closer to the real CN, and the overall REMS decreases. The simulation diagram illustrating the construction of build sets is shown in Fig. 3.

Table 2. Summary of results for predicted CN

Data Source	Total compounds	Furanic compounds	
	Root mean square error	Root mean square error	Maximum absolute error
Core Data	5.97CN	7.60CN	18.78CN
Expanded Data	5.95CN	3.86CN	7.52CN

The cetane values of seven furan compounds were predicted by the artificial neural network model, and compared with the data obtained from the experiment, the results show that the overall RMSE of the model based on the core data set was 7.60 CN units with the maximum absolute error was 18.78 CN, which is less than satisfactory. So, an expanded data set was created by adding experimental results for six of the seven furanic compounds to the core data, and the network is retrained using this expanded data set by the same way. The average absolute error between experimental and predicted cetane numbers for the furanic compounds improved to 3.86 CN units, with a maximum absolute error of 7.52 CN units. This represents an improvement of 49.21% when using the expanded data set over the core data set. This validates the hypothesis that a targeted expansion of the input data set can extend the applicability of the model to new molecular classes.

After verification, the model was able to predict CN for other molecules, including furanic compounds, biomass-derived hydrocarbons, and fatty acid methyl esters within a 95% confidence interval for the biofuel species for which reliable published values could be found. It shows that QSPR model based on artificial neural network provides a convenient and reliable way to predict the novel fuel properties and determine the CN value of some compounds. Compared with direct measurement, the efficiency of finding new fuel with target cetane value is greatly improved, which provides a strong support for the research of biomass fuel.

Qin et al. [49] established a quantitative structure-property relationship model of organic mixtures to predict the flash point of binary organic mixtures based on artificial neural network. Flash point (FP) refers to the lowest temperature at which the vapor pressure of a liquid corresponds to a combustible concentration, and is usually used to characterize the danger of a liquid's susceptibility to fire and explosion [50]. The flash point of flammable organic liquids has been studied widely. It is very easy to determine the flash point of a single component organic liquid, which can be find easily from literature or database. However, the actual work encountered more liquid organic mixtures. Empirical formula method is a relatively common prediction method. Bao et al. [51] predicted mixed solution flash point based on the saturated vapor pressure of pure components, Raoult's law and gas-liquid equilibrium theory. Using Le Chatelier equation and Antoine equation to derive flash points of binary mixture. Yang et al. [52] used Taylor polynomials to fit the empirical formulas of flash point and spontaneous combustion point of binary mixed liquid composed of alcohol, ketone, ether and ester under normal pressure. But most of the empirical formulas are used to determine binary mixtures, and the empirical parameters need to be determined according to different substances. Due to the complexity of mixtures, high cost of analytical methods, limitation of experience parameters, the empirical formula method cannot be widely used, the prediction of flash points in liquid organic mixtures is still a difficult task [53,54].

In this study, flash point QSPR models of 288 binary organic mixtures were established based on RBF neural network. Experimental flash point values of the studied samples were obtained from references [55]. An electro-topological state index (ETSI) [56,57], which has been widely used in QSPR research, is used as the descriptor of the mixture (the independent variable of the model). The descriptors of mixtures were established by weighted summation of 9 elements in the ETSI parameters of 18 compounds.

The five ETSI parameters screened by stepwise regression were used as input variables to establish a new RBF neural network with a structure of 5-37-1, i.e., 5 input layer nodes, 37 hidden layer nodes and 1 output layer node, FP variables. The 288 mixed samples were divided into two groups. The first group was composed of 255 mixed samples for the training of neural networks, and the second group contained 73 mixed samples as the test group. The prediction performance of the developed model is also

evaluated by k-fold cross validation [58]. In the design of RBF neural network, the center and width of basis function are selected first, and then the weight of connections between neurons is optimized. Random sampling and k-means method are commonly used to select the center of the basis function. Pseudo-inverse algorithms are used to form the weights of connections between neurons in the hidden layer and the output layer. The error function RMSRE is used to monitor and control this learning process.

After the training of the RBF-ANN model, the network parameters with minimum RMSRE value are obtained. The flash points of 73 mixtures in group II were predicted using the established neural network model, and the predicted flash points were plotted against the experimental values, as shown in Fig. 4. The RMSRE of the FP prediction of the 73 mixtures was 1.86, with an average relative error of 1.44%. In the k-fold cross validation, the predicted RMSRE of flash point values of 215 mixtures in group I was 1.11, with an average relative error of 0.87%, which is also shown in the figure. The results show that applied RBF-ANN model with ETSI, stepwise regression are promising methods to establish QSPR of FP values for binary organic mixtures.

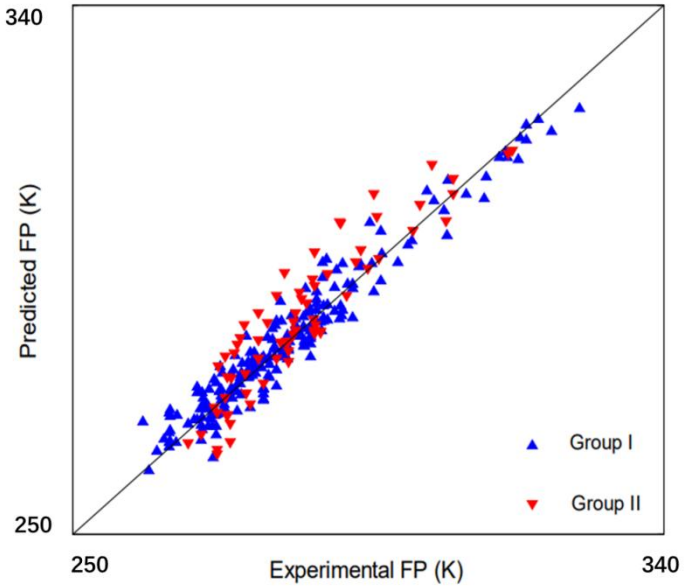

Fig. 4. Plot of predicted versus experimental values of RBF-ANN 1[49]

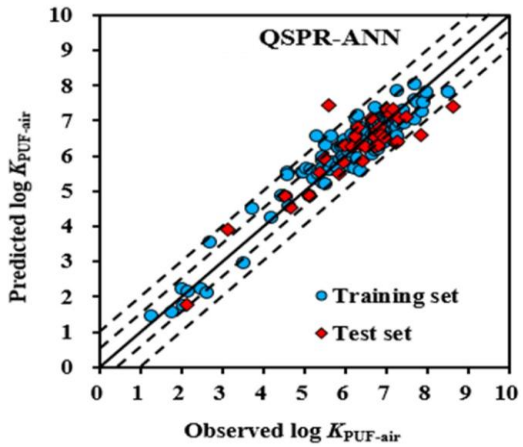

Fig. 5. Plots of the predicted versus observed for log $K_{PUF-air}$ by QSPR-ANN [59]

Zhu et al. [59] exploring QSPR models for predicting PUF-air partition coefficients of organic compounds with ANN approaches. In this study, 6 descriptors were selected for QSPR model construction and through the back propagation-learning algorithm, ANN-QSPR model was evaluated by the SPSS software. The models are confined to 6-3-1 structure, which considered the three hidden nodes (parameter size) and the learning rate of 0.01 (parameter). As shown in Fig. 5, the prominent character for developed ANN model showed satisfactory goodness-of-fit in the observed and predicted log $K_{PUF\text{-}air}$, which demonstrate the ANN-QSPR model occupied preferable prediction performance and can be used as an efficient tool to predict log $K_{PUF\text{-}air}$.

Adriel et al. [60] used a combined ANN-QSPR methodology to model the mixing energy of solutions using COSMO molecular descriptors. A three-layered feedforward ANN was used in this work. The hyperbolic tangent was selected as the activation function for each neuron in the hidden layer. While, for the input layer, a linear activation function was set. The ANN-QSPR procedure was successfully applied for the prediction of model parameters based on deduced molecular descriptors. The estimations of mixing enthalpies are in good agreement with experimental data, showing RMSE□(26.27, 32.9)/J·mol^{-1}. Hassanzadeh et al. [61]. applied a combination of RBFN and GA to build a quantitative structure-property relationships model to predict the adsorption coefficients of 40 small molecules on the surface of multi-walled carbon nanotubes. RBFN is used to construct QSPR model and GA is used to optimize the numerical values of RBFN centers. The accuracy and predictive ability of the model evaluated using internal and external procedures are satisfactory, providing a powerful tool in the research of the adsorption mechanism of organic compounds on carbon nanotubes.

4. CONCLUSION AND RECOMMENDATION

As a kind of nonlinear model, Artificial neural network has unique learning ability and automatic modeling function, and has extremely high solving ability for nonlinear problems. Its' fitting effect is obviously better than that of previous multiple linear models. Quantitative structure-property study is currently one of the most active fields of application of artificial neural network. The combination of the artificial neural network model and the QSPR method, has important significance in the analysis of the biomass fuel, prediction of the risk of dangerous chemical properties (such as flash point, ignition point, etc.), the estimation of thermodynamic properties (such as heat generation and formation enthalpy, etc.) and the study and prevent of the harm of industrial poisons.

In the process of application, researchers found that the directional expansion of the original data set of molecular physicochemical properties can make the neural network model better applied to the research target field. And the screening of molecular descriptors with higher correlation with the results by means of stepwise regression can make the convergence rate of neural network faster and improve the prediction accuracy.

However, the "black box" problem of artificial neural network model and over fitting problem makes some obstacles in the application process. The improvement of these problems depends on developments in neuroanatomy and related mathematic and the accumulation of the application experience. At the same time, the quantitative description of mixtures has been a difficult problem in QSPR research for a long time. The current QSPR research still lacks effective descriptors to describe the chemical information of mixtures. It is also important to consider how to choose and obtain more accurate molecular descriptors and establish a more broadly applicable ANN-QSPR model of mixtures.

DISCLAIMER

The products used for this research are commonly and predominantly use products in our area of research and country. There is absolutely no conflict of interest between the authors and producers of the products because we do not intend to use these products as an avenue for any litigation but for the advancement of knowledge. Also, the research was not funded by the producing company rather it was funded by personal efforts of the authors.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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