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A QSAR Study towards Predicting the Adsorption of Environmental Pollutants by Multi-Walled Carbon Nanotubes

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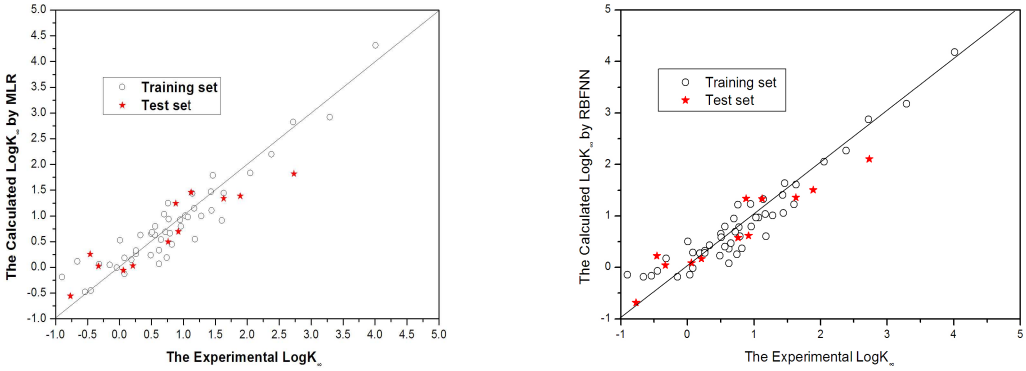
Abstract: Nanotechnology has led to the development of new materials with unique properties and a wide variety of applications. Meanwhile, it has raised great concerns regarding their properties and potential adverse effects to humans and the environment. In this work, a Quantitative Structure-Activity Relationship (QSAR) modeling study was carried out for predicting the adsorption property of a set of 59 environmental pollutant aromatic compounds into multi-walled carbon nanotubes. We report a systematic evaluation of multiple linear regression (MLR) and artificial neural network (ANN) methods along with a variety of structure representations and feature selection algorithms. Judging from the attained statistical results, our derived QSAR models have an acceptable overall accuracy and robustness, as well as good predictivity on external data. This QSAR study suggested also that the adsorption ability of these compounds is mainly explained by size, charge and hydrophobicity factors. Moreover, it showed to be a simple, precise and credible tool forward-predicting the adsorption of aromatic compounds by multi-walled carbon nanotubes.

Keywords: Environmental Pollutants, Multi-walled Carbon Nanotubes, Quantitative Structure-Activity Relationships (QSAR); Multiple Linear Regression (MLR); Artificial Neural Networks (ANN)

Graphical Abstract:



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2D-QSAR modeling was performed on the adsorption property of a set of 59 environmental pollutions aromatic compounds into multi-walled carbon nanotubes by MLR and RBFNN.

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Introduction:

QSAR studies forward-modeling nanomaterials are still in an early stage. Many research efforts now aim at a better understanding of the properties and behavior of nanomaterials (including nanoparticles). As a desire for contributing to the use of the QSAR methods to tackle nanomaterials, we will present the development of 2D-QSAR models based on a series of aromatic compounds known to adsorb on MWCNTs.

Materials and Methods:

A data set of 59 aromatic compounds with the adsorption parameter K_∞ was used as dependent variable after log-transforming ($\log K_\infty$) to be of practical use in the following QSAR modeling. All molecular structures were drawn and energetically optimized by molecular mechanics MM^+ and the semi-empirical PM3 and MOPAC, then were brought into the CODESSA program to calculate five kinds of descriptors. The MLR and ANN were then used to build and validated the models.

Results and Discussion:

The best-fit linear regression model found using four descriptors is given below along with its MLR statistical parameters.

$$\mathrm{Log}K_\infty = 5.002\times10^{-3}GI + 5.262E_{\mathrm{min}}^{\mathrm{C\text{-}H}} - 4.084RNN - 5.456Q_{\mathrm{max}} - 32.596$$

N = 47, R^2 = 0.886, RMS = 0.3374, F = 351.71, ρ = 11.75

In this equation, GI stands for the gravitation index (all bonds), $E_{\mathrm{min}}^{\mathrm{C\text{-}H}}$ for the minimum exchange energy for a C-H bond, RNN represents the relative number of N atoms, and Q_{max} is the maximum partial charge. For the discussion of the descriptors, one can conclude that small, less charged compounds are expected to be adsorbed more favorable by these nanomaterials. Prediction results were obtained using the external test set (N = 12). In this case, the obtained statistical parameters were the following: Q^2 = 0.894, RMS = 0.3654, F = 75.01. The training quality and the predicting ability of the RBFNN model can be judged from the obtained statistical results, *i.e.* for the training set (N = 47): R^2 = 0.906, RMS = 0.2903, F = 403.84; and for the external test set (N = 12): Q^2 = 0.894, RMS = 0.3654, F=75.01.

A Williams plot, *i.e.* a plot of the standardized cross-validated residuals *vs.* leverage values (or hat values, $h = 3m/n$, for this study, m = 4, n = 47) can be used for an immediate and simple graphical detection of both the response outliers and structurally influential chemicals in the model.

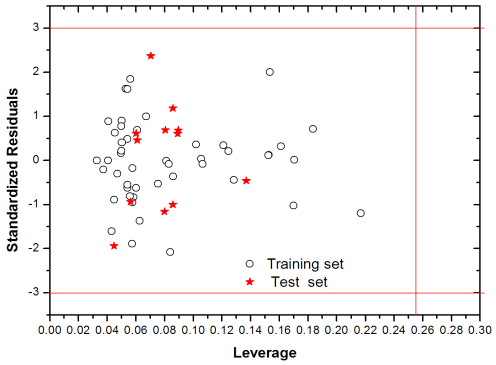

Fig. 1. The William plot for the training and test sets.

Conclusions:

QSAR models (MLR analysis and RBFNN) have been developed to predict the adsorption of aromatic compounds by multi-walled carbon nanotubes. The acceptable statistical results of both these models proved their robustness as well as their predictive power. In addition, the developed MLR model provided some useful insights regarding which descriptors are most related to the adsorption ability of the analyzed compounds, suggesting that to be mainly governed by size, hydrophobic and charge factors.

References:

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