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In silico toxicity prediction of phenol derivatives with ISIDA descriptors using multiple linear regression and machine learning approach

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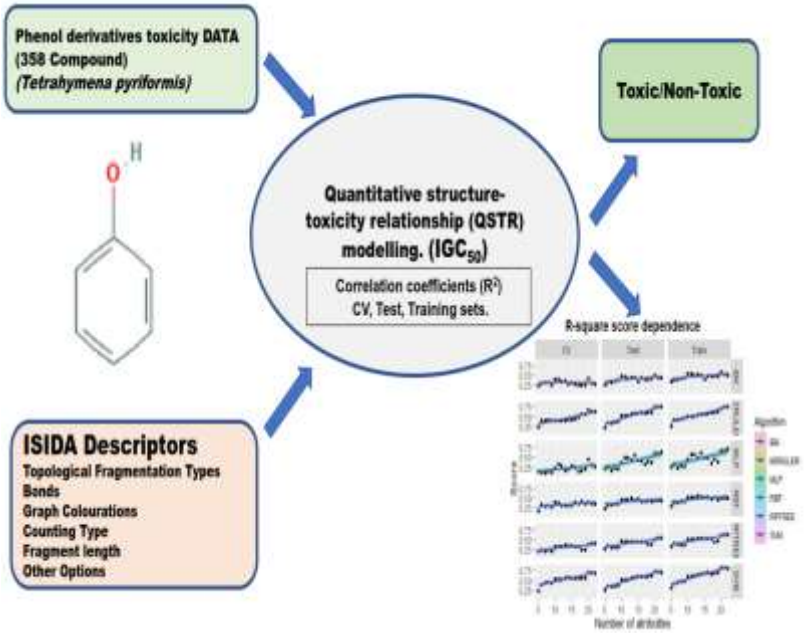
Graphical Abstract



Abstract.

Phenolic compounds are considered as dangerous pollutants, which produces serious environmental problems by pollution of water streams because of their great water solubility and high toxicity. In this paper we present the modeling of inhibitory grown activity against Tetrahymena pyriformis with structural feature descriptors. Quantitative structure-toxicity relationship model for acute toxicity of phenol derivatives was performed using Multiple Linear Regression (MLR), Reduced Error Pruning Tree (REPTree), M5 Model Rules (M5R), Multilayer Perceptron (MLP), Instance-Based Learning algorithms using K nearest neighbor (IBk-ANN), Support vector machine (SVM), and Radial basis function network (RBF). The correlation coefficients (R^2) of training sets and test sets were 0.88 and 0.86 for the best MLR model, 0.82 and 0.72 for the best machine learning model (SVM), respectively. Following to the obtained results, our proposed model may be useful to predict of toxicity and risk assessment of phenol derivatives compound.

Keywords: Phenolic compounds; acute toxicity; *Tetrahymena pyriformis*; structural feature descriptors; Support vector machine

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