

QSPR models for predicting the impact sensitivity of explosives

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The development of explosives focuses on research in order to secure both the desired explosive performance and insensitivity according to the change in chemical structures. As the performance and insensitivity of explosive tend to be inversely proportional, it takes a lot of time and money to develop insensitive explosive. QSPR (Quantitative Structure Property Relationship) method is an efficient method to predict the sensitivity of new explosives prior to synthesis and impact testing. The purpose of the study is to develop a QSPR model that can predict the impact sensitivity of new explosives. For 285 compound data, the Tanimoto coefficients, calculated from Avalon Fingerprint, were structurally varied into training data(171) and test data(114). The forward selection method, genetic algorithm, and recursive feature elimination method were used for the feature selection method of the model development, and MLR, SVM, RF and GBT models were used as the algorithms. The optimized QSPR model to predict impact sensitivity is expected to greatly contribute to technological advances for developing insensitive explosives.