Rapid and Accurate Estimation of Densities of Energetic Salts by Using QSPR Method

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***Abstract*:** *Energetic salts often have higher densities, thermal stability than similar nonionic molecules. Densities of energetic materials plays a key role in evaluating explosive performance. Experimental determination of density is not only time-consuming and expensive, but also inherently difficult to synthesize and test in the laboratory. In this study, quantitative structure-property relationship (QSPR) was developed for predicting the densities of from 2D chemical structure. Cations and anions were respectively parameterized using PreADMET program. Multiple linear regression (MLR) and support vector machine (SVM) are used in conjunction with bootstrapping and forward selection method to select best subset of descriptors related to their densities. All models were evaluated by internal validation using bootstrap method, external validation, y-scrambling and applicability domain. The consensus models were tried to improve the predictive power of each model. These models will provide the important research tools for exploring the design of novel energetic salts.*

Keywords: *Energetic salts, QSPR, density*