A New Estimation Algorithm of Physical Properties based on a Group Contribution and Support Vector Machine

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A new method for the predicting the physical property was proposed to predict 15 physical properties for the chemicals which consist of C, H, N, O, S and Halogens. This method was based on the group contribution method that was oriented from the assumption that each fragment of a molecule contributes a certain amount to the value of its physical property.
In order to improve the accuracy of the prediction of the physical properties and the applicability, we extended the database significantly modified the existing group contribution methods and then established a new method for predicting the physical properties using Support Vector Machine (SVM) which is a statistical theory and has never used for predicting of the physical properties. The newly proposed method can play a crucial role in the estimation of new compounds in terms of the expenses and times.