Development of Predictive Web-Program for Physicochemical Properties by QSPR Approach

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***Abstract*:** *The aim of this study is to develop predictive web-program for QSPR model of physicochemical properties. First of all, we constructed the QSPR model for predicting auto-ignition temperature (AIT) and heat of sublimation (HOS) of diverse organic compounds. This two models were developed from HOS data of 626 organic compounds and AIT data of 923 organic compounds, respectively. The best models of both two kinds of QSPR model are consensus model and the performance of best models is R^2=0.730 RMSE=59.076 MAE=48.240, R^2=0.783 RMSE=13.289 MAE=9.447, respectively. Secondly, we developed the predictive web-program for QSPR models. The web-program was developed by using JAVA program language and we applied the MarvinSketch program for inputting structure of organic compounds. The two QSPR models which were applied in web-program are running via RapidMiner program. And we used JSP for treatment of organic compounds structure and predicted values which were calculated from the QSPR model.*

Keywords: *QSPR, Auto-ignition temperature, Heat of sublimation, Program*