

Theoretical Prediction of the Complex P-Glycoprotein Substrate Efflux Based on the Novel Hierarchical Support Vector Regression Scheme

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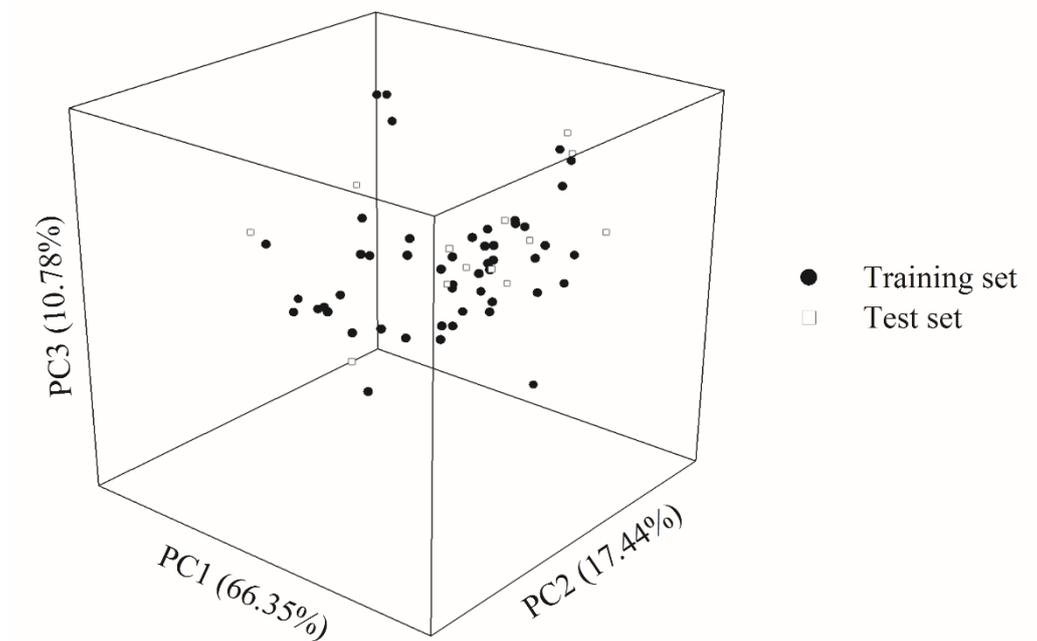
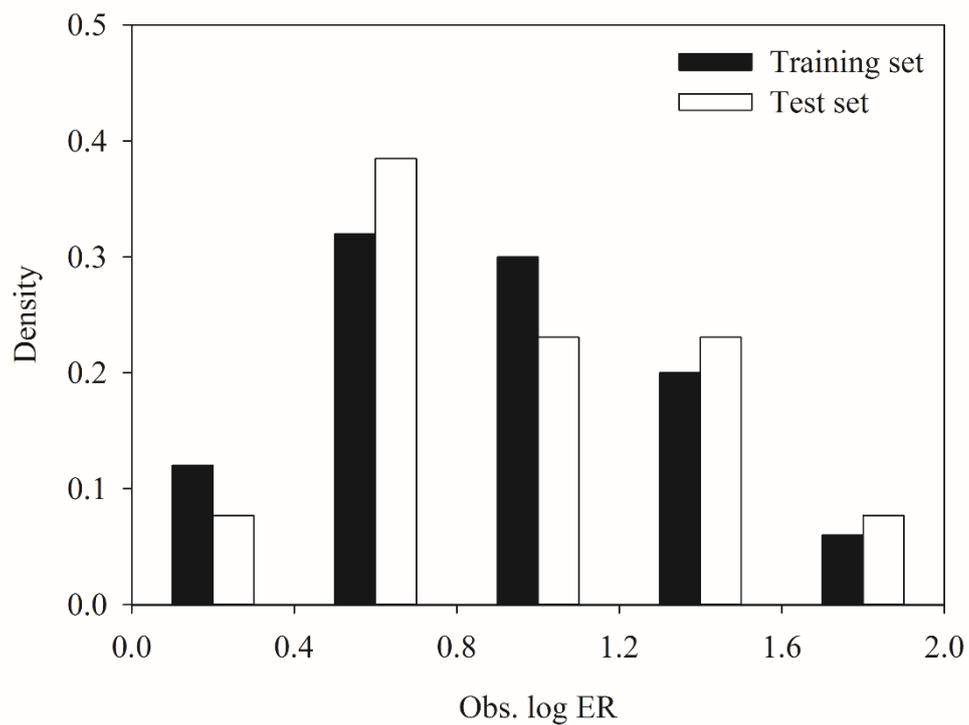
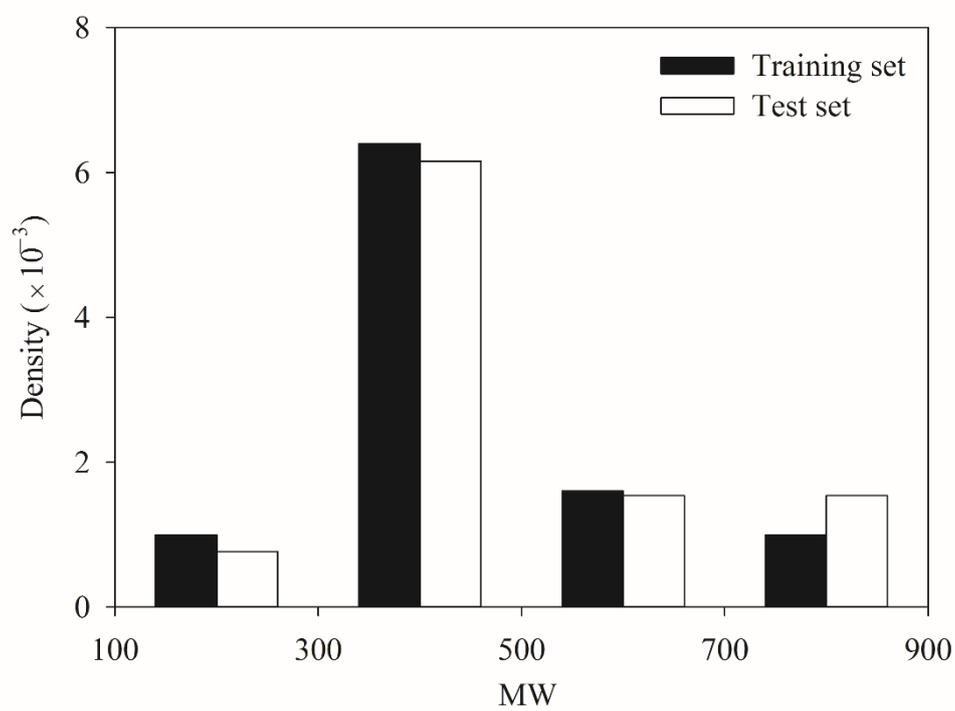


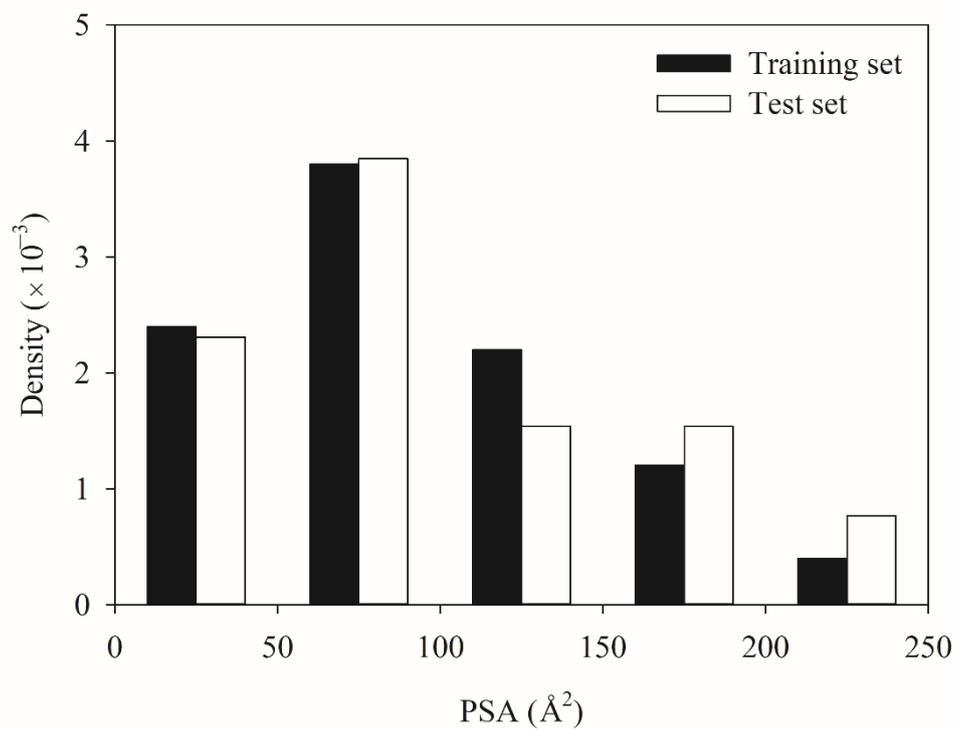
Figure S1. Molecular distribution for the samples in the training set (solid circle) and test set (open square) in the chemical space spanned by three principal components.



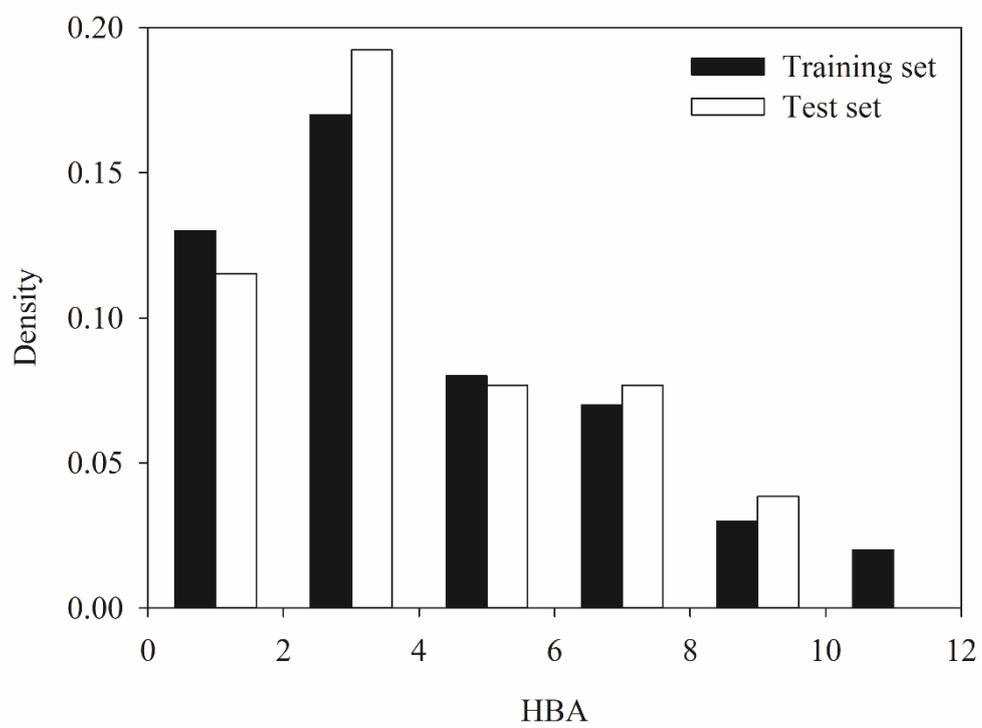
(A)



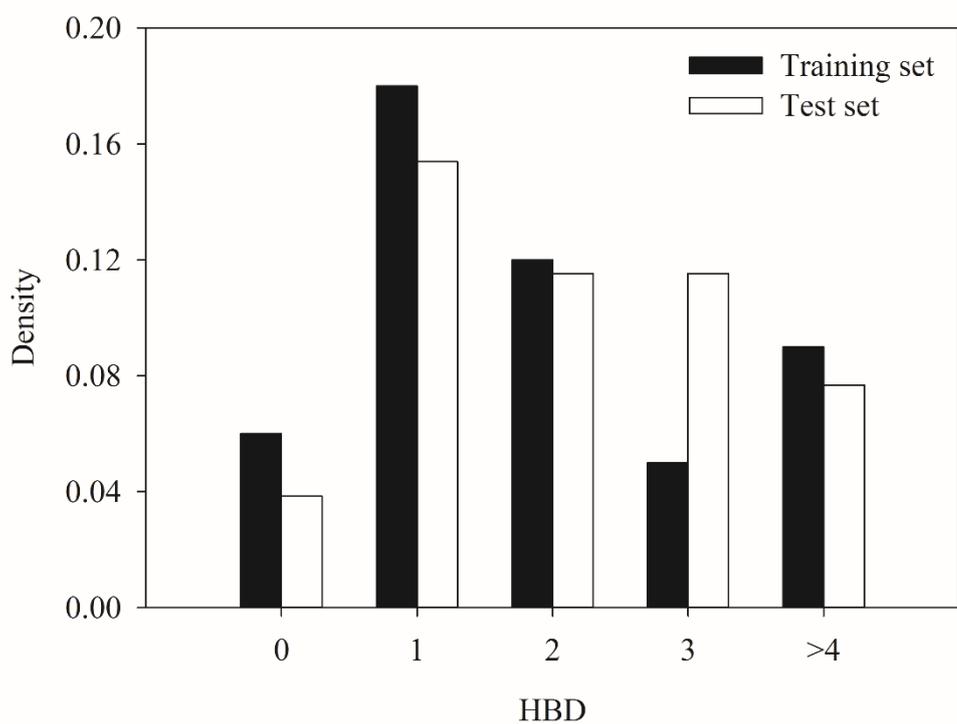
(B)



(C)



(D)



(E)

Figure S2. Histograms of (A) observed log ER, (B) molecular weight (MW), (C) polar surface area (PSA), (D) number of hydrogen bond acceptor (HBA), and (E) number of hydrogen bond donor (HBD) in density form for all molecules in the training set and test set.