

In Silico Prediction of Skin Permeability Using a Two-QSAR Approach

Supporting information

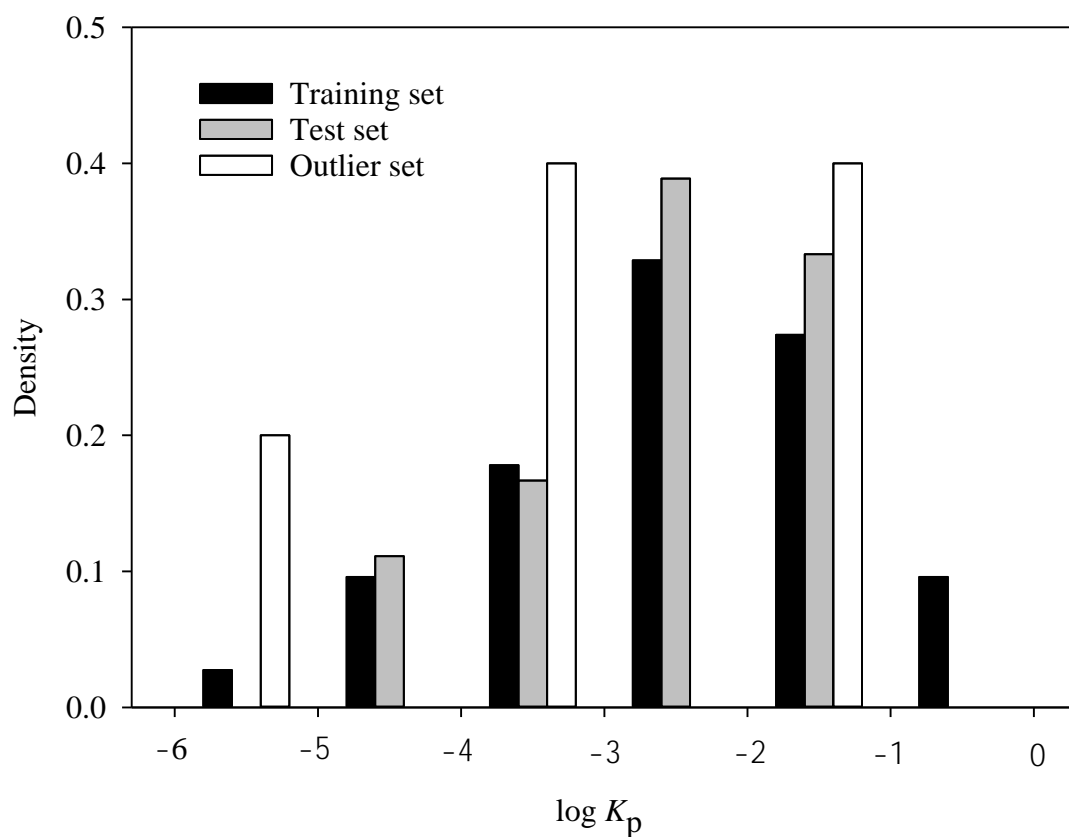
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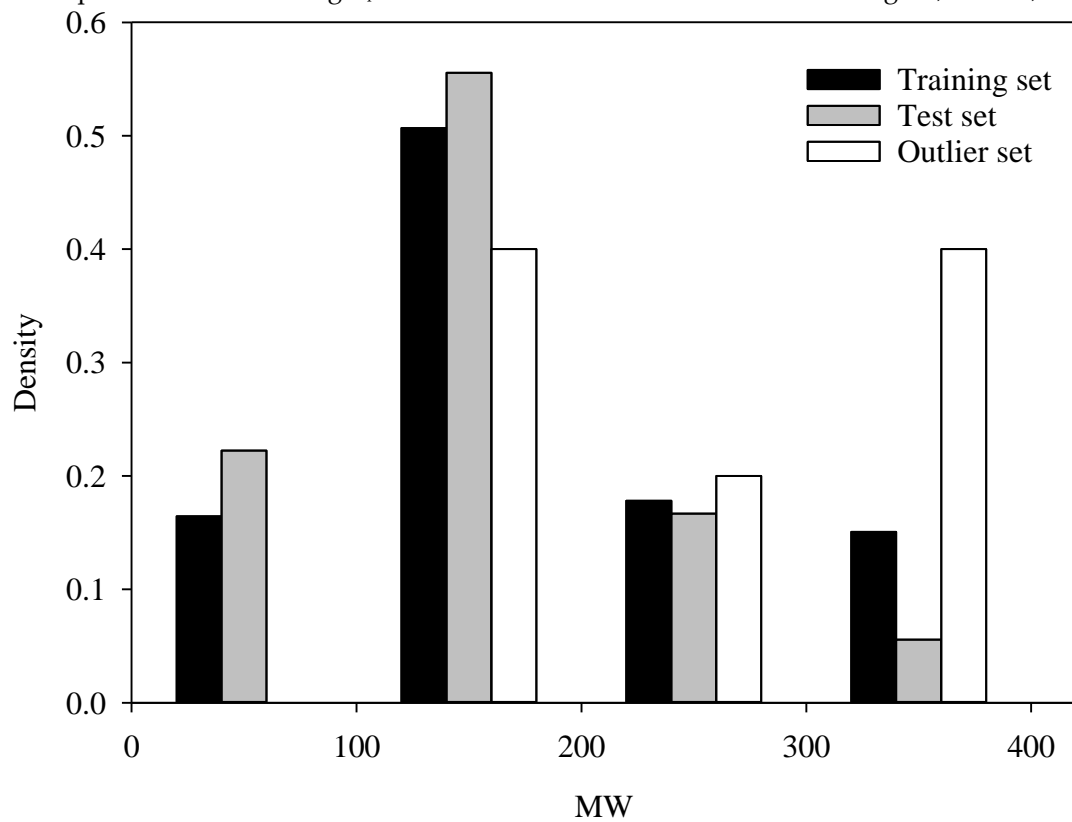
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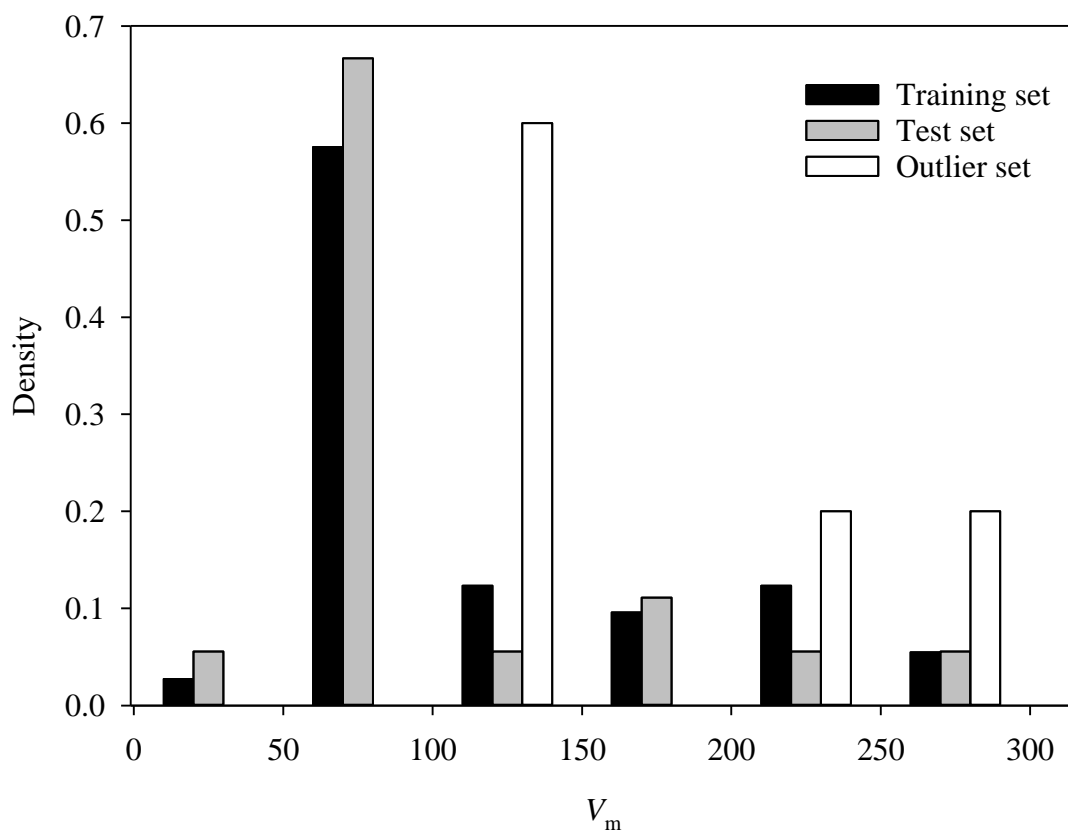
Equal contribution as first authorship



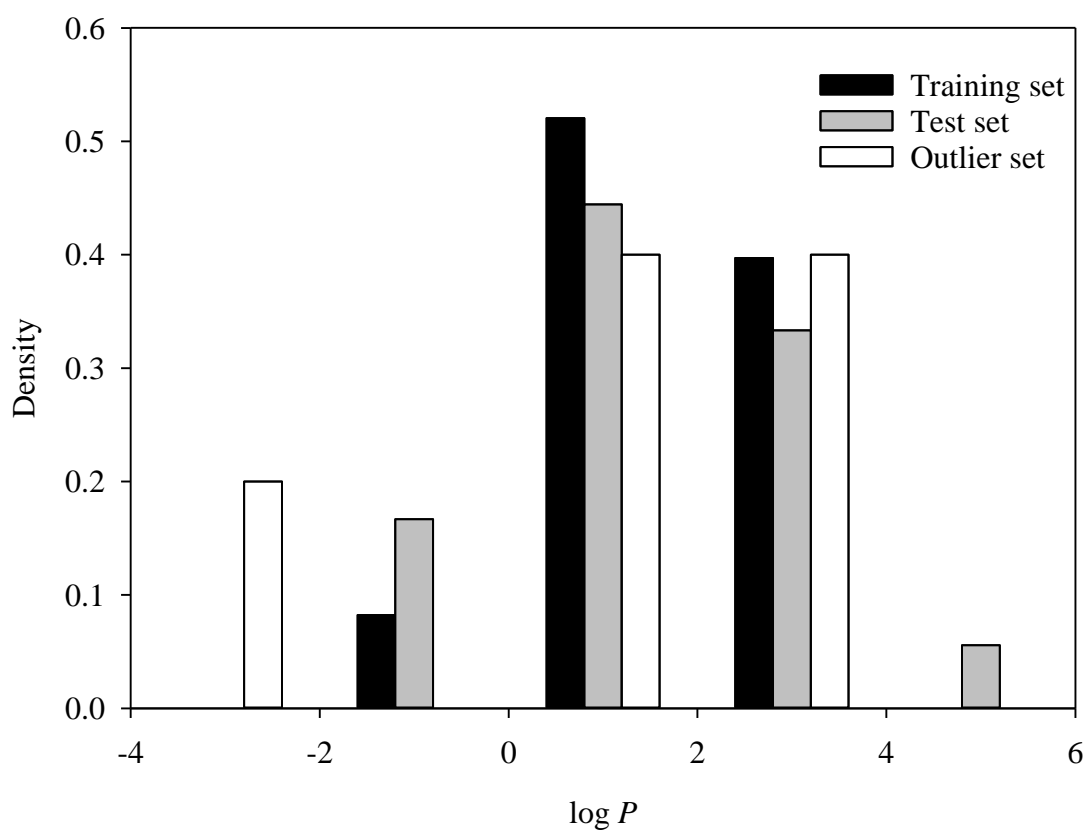
(A) Histogram representation of the $\log K_p$ distribution for all molecules in the training set, test set, and outlier set.



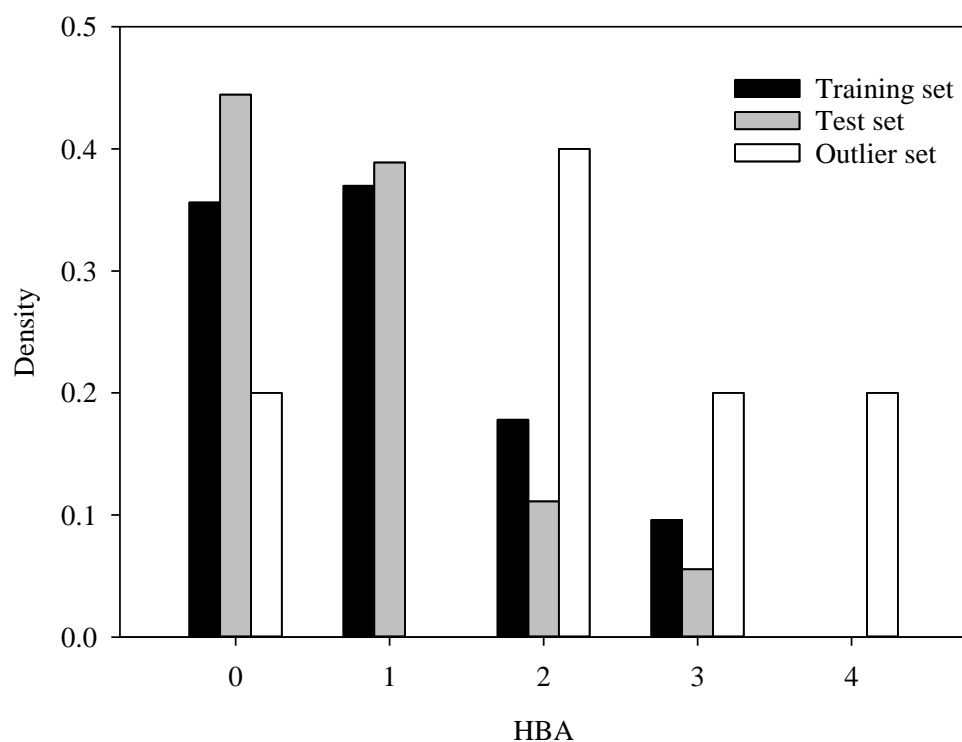
(B) Histogram representation of the molecular weight (MW) distribution for all molecules in the training set, test set, and outlier set.



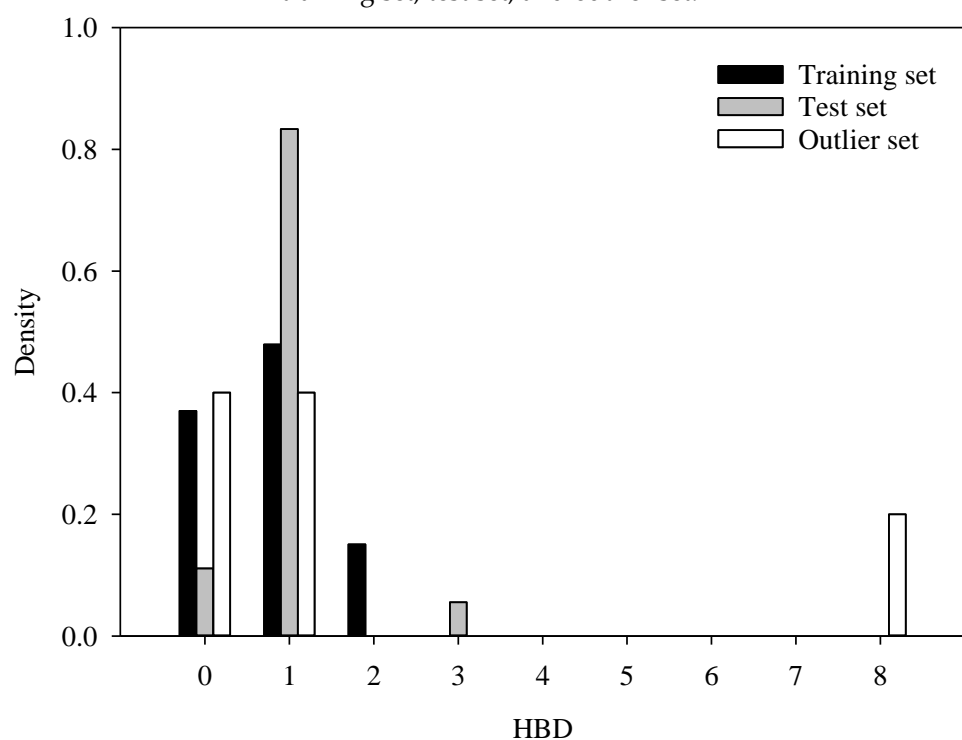
(C) Histogram representation of the molecular volume (V_m) distribution for all molecules in the training set, test set, and outlier set.



(D) Histogram representation of the n -octanol-water partition coefficient ($\log P$) distribution for all molecules in the training set, test set, and outlier set.



(E) Histogram representation of the number of hydrogen bond acceptor (HBA) distribution for all molecules in the training set, test set, and outlier set.



(F) Histogram representation of the number of hydrogen bond donor (HBD) distribution for all molecules in the training set, test set, and outlier set.

Figure S1. Histogram representation of the distributions of various descriptors for all molecules in the training set, test set, and outlier set.