

(A)



(B)



(C)



(D)



(E)



(F)



(G)

Figure 1.Histogram representation of the distributions of various descriptors for all molecules in the training set, test set, and outlier set. (A) log *P*e, (B) molecular weight (MW), (C) log *P*, (D) log *D*, (E) polar surface area (PSA), (F) fractional polar surface area (FPSA), and (G) dipole moment (*μ*).