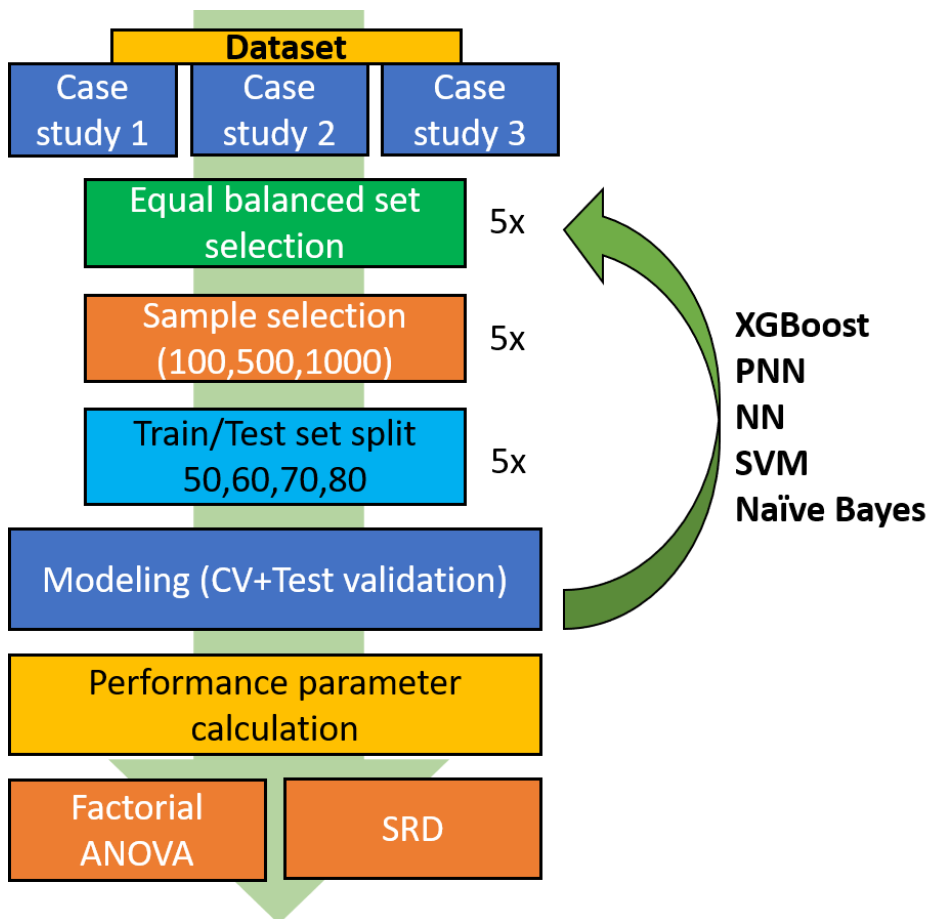


Effect of Dataset Size and Train/Test Split Ratios in QSAR/QSPR Multiclass Classification

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(a)



(b)

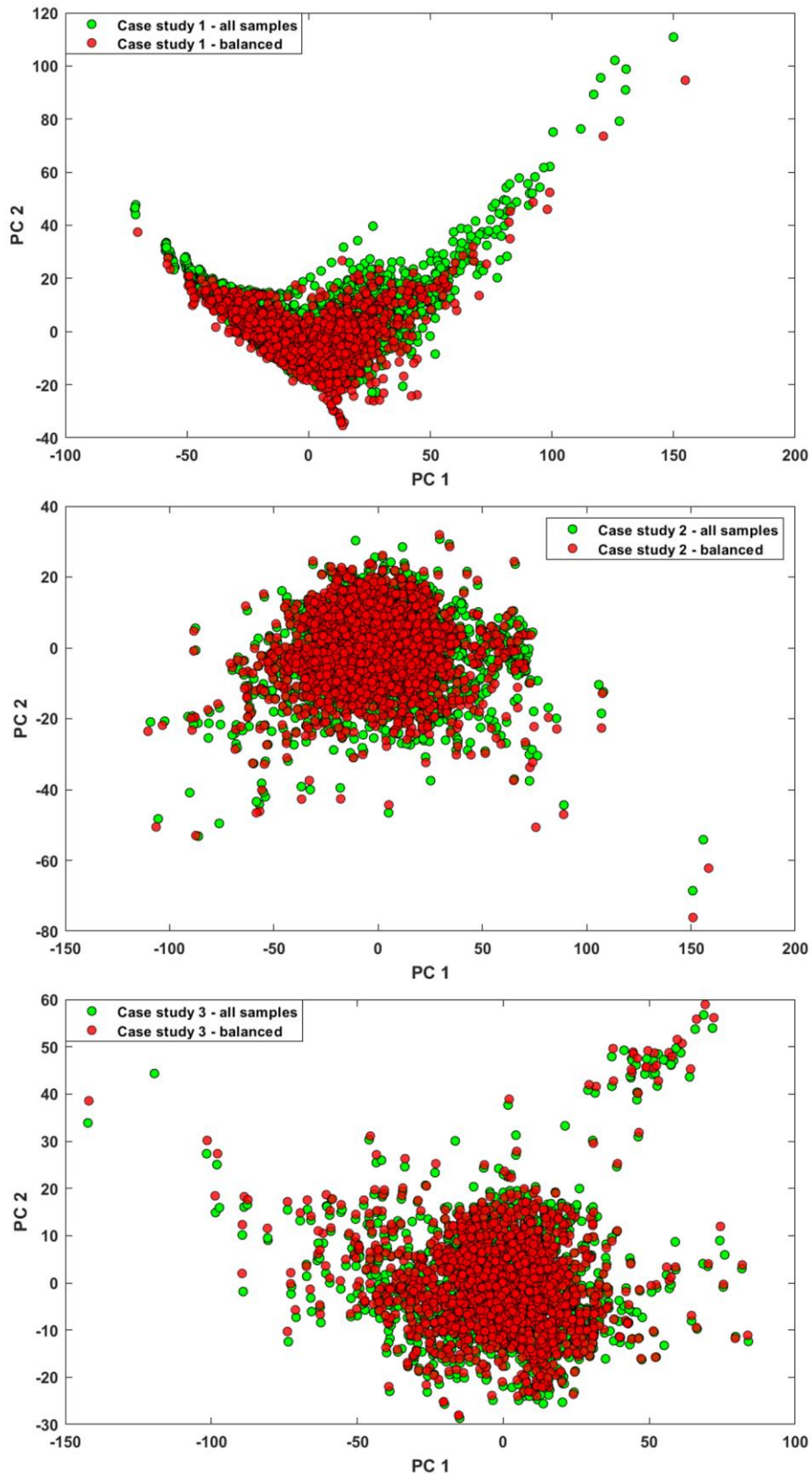


Figure S1. The applied modeling workflow (a). Principal component analysis (PCA) score plots (b).