



Figure S1. Chemical space of the training and external test sets. A. Comparison of logP and molecular weight (MW) values of the training set' inhibitors and non-inhibitors. B. Comparison of logP and MW values of the test set' inhibitors and non-inhibitors. C. PCA of the training set' inhibitors and non-inhibitors. D. PCA of the test set' inhibitors and non-inhibitors.