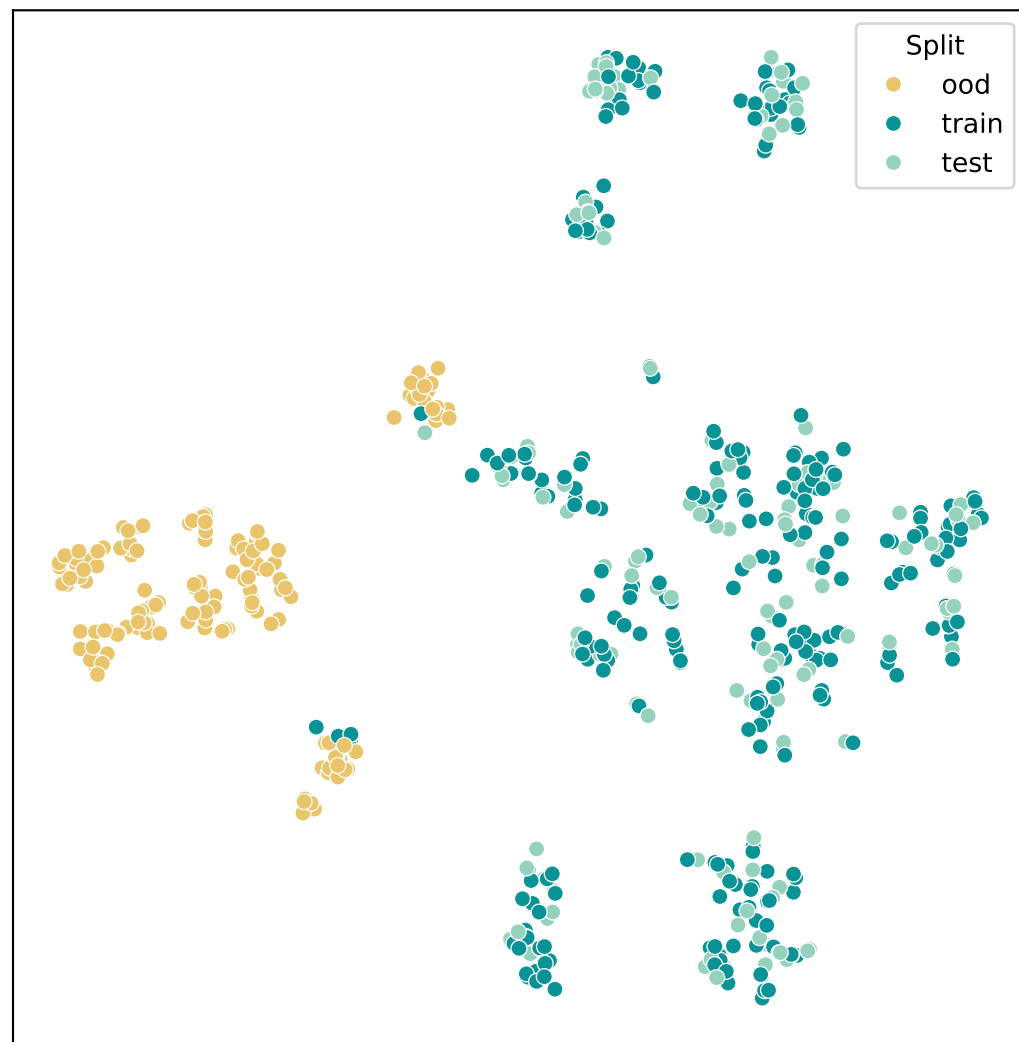
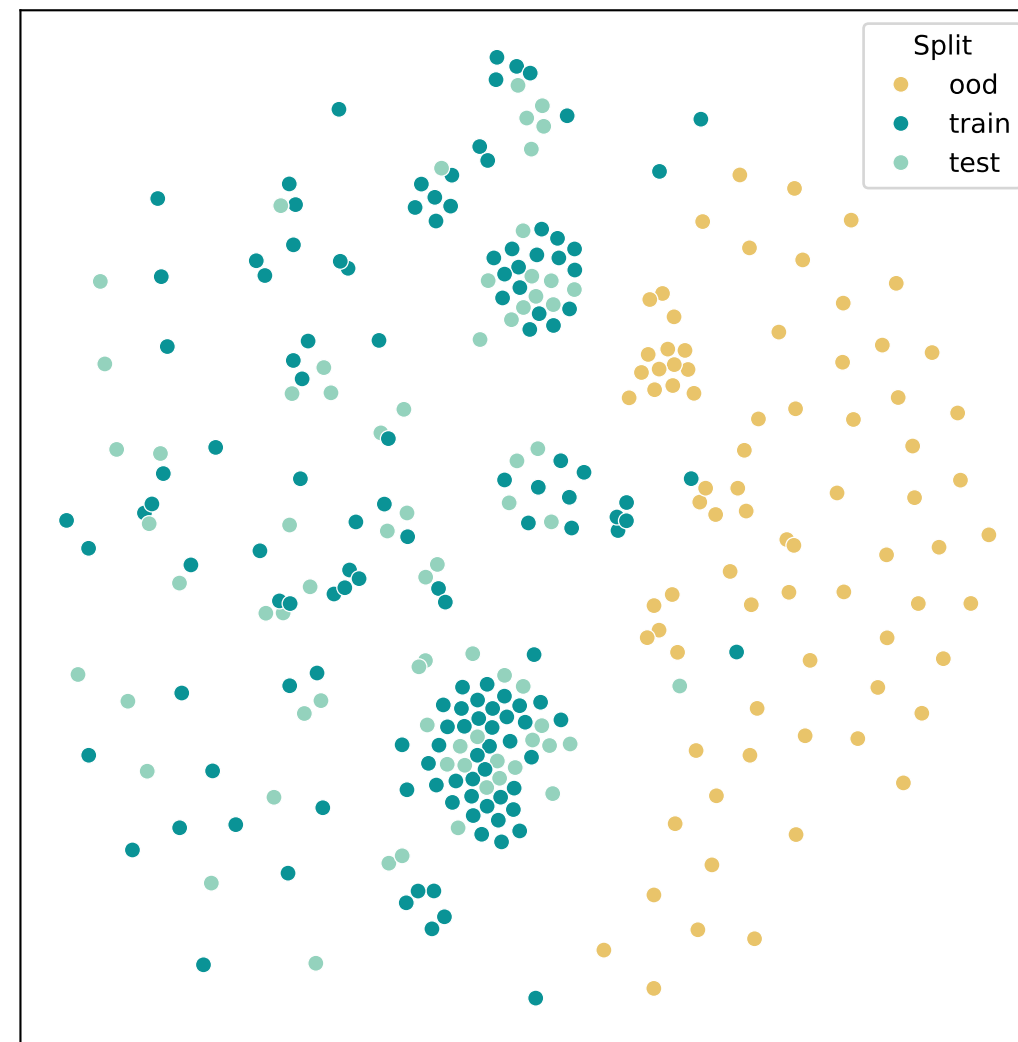


TSNE of CHEMBL2835_Ki (n=613)



Whole molecule ECFPs



Cyclic skeleton ECFPs