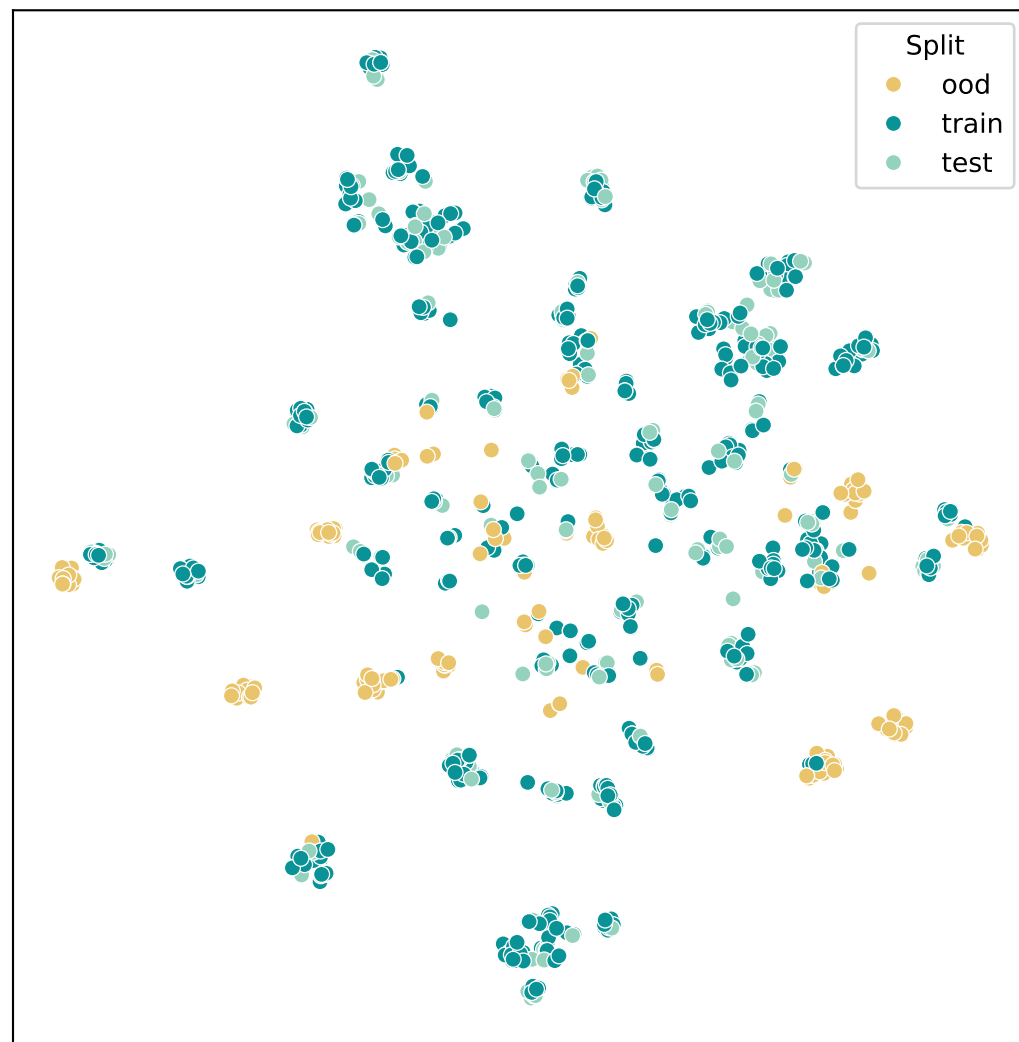
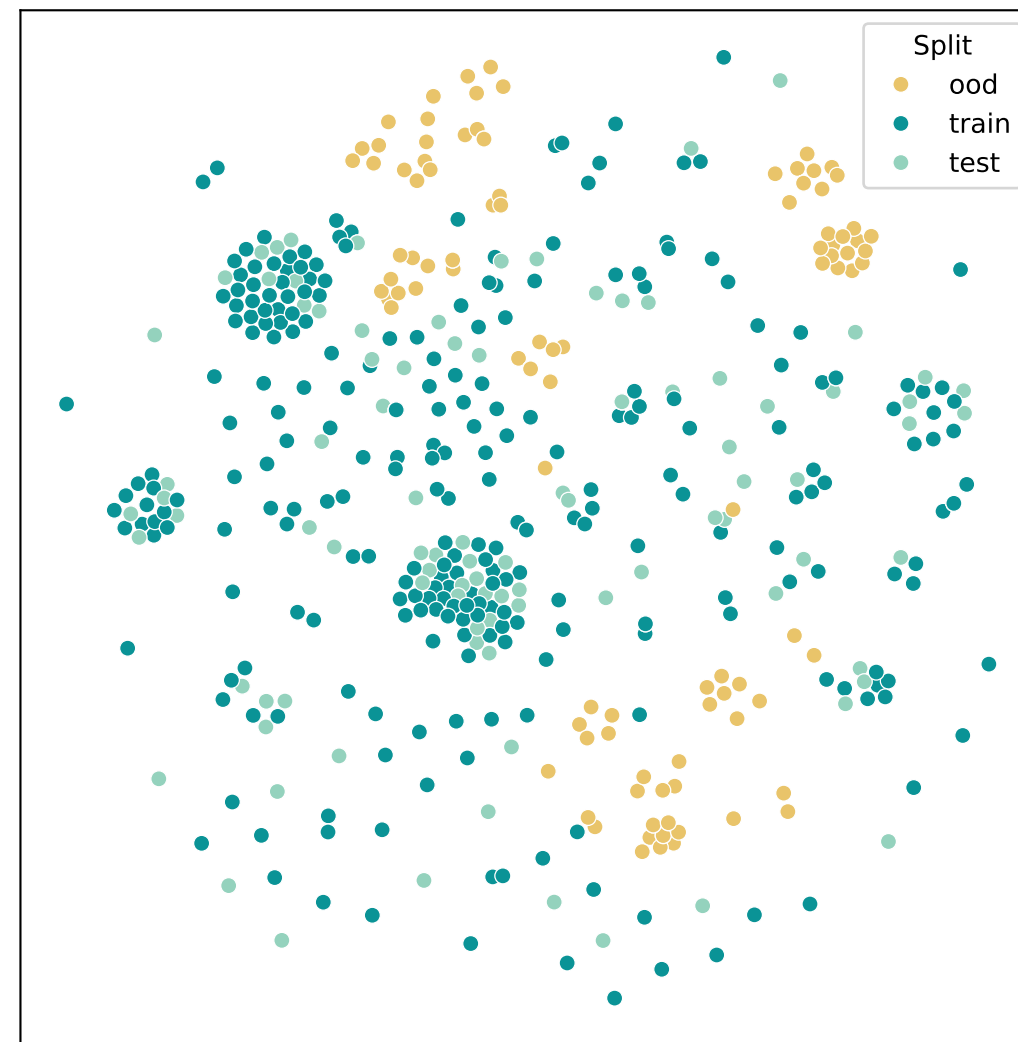


TSNE of CHEMBL3979_EC50 (n=1109)



Whole molecule ECFPs



Cyclic skeleton ECFPs