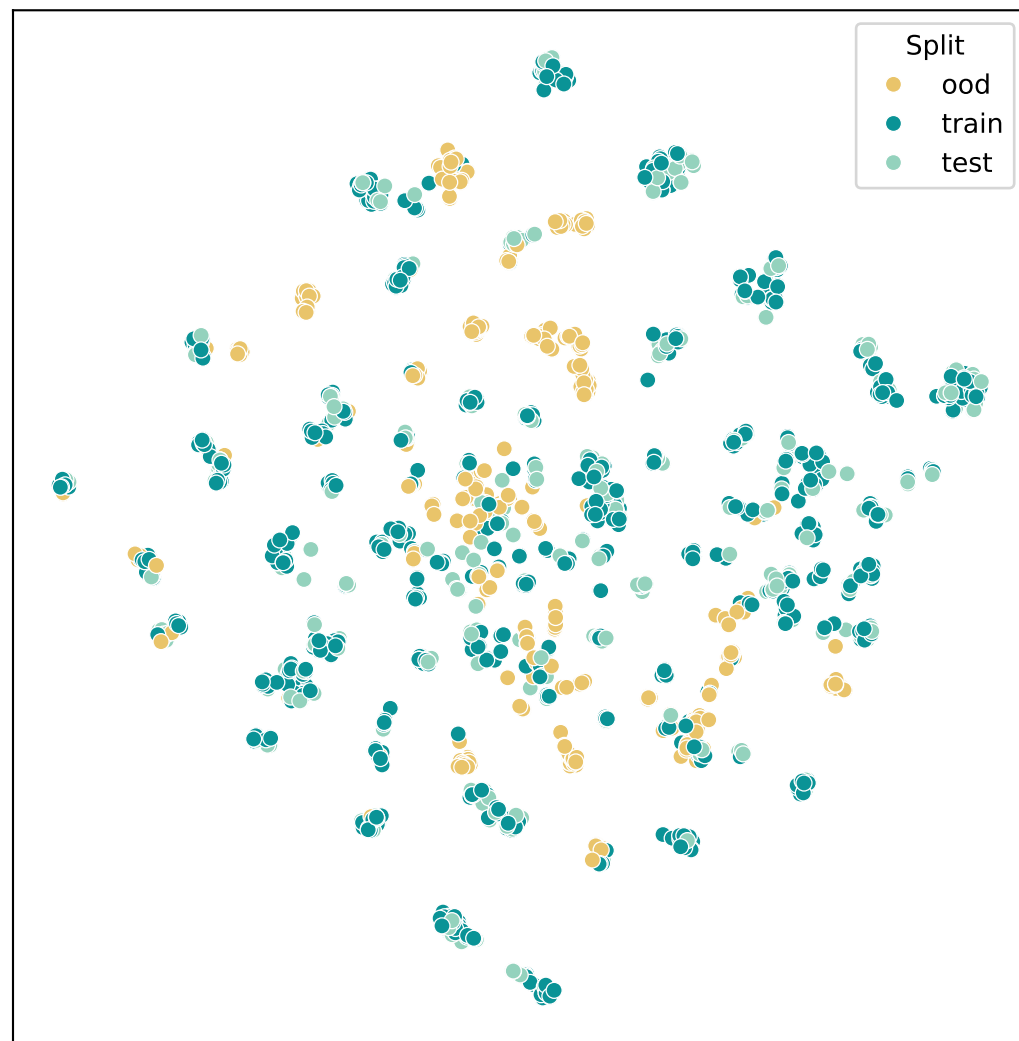
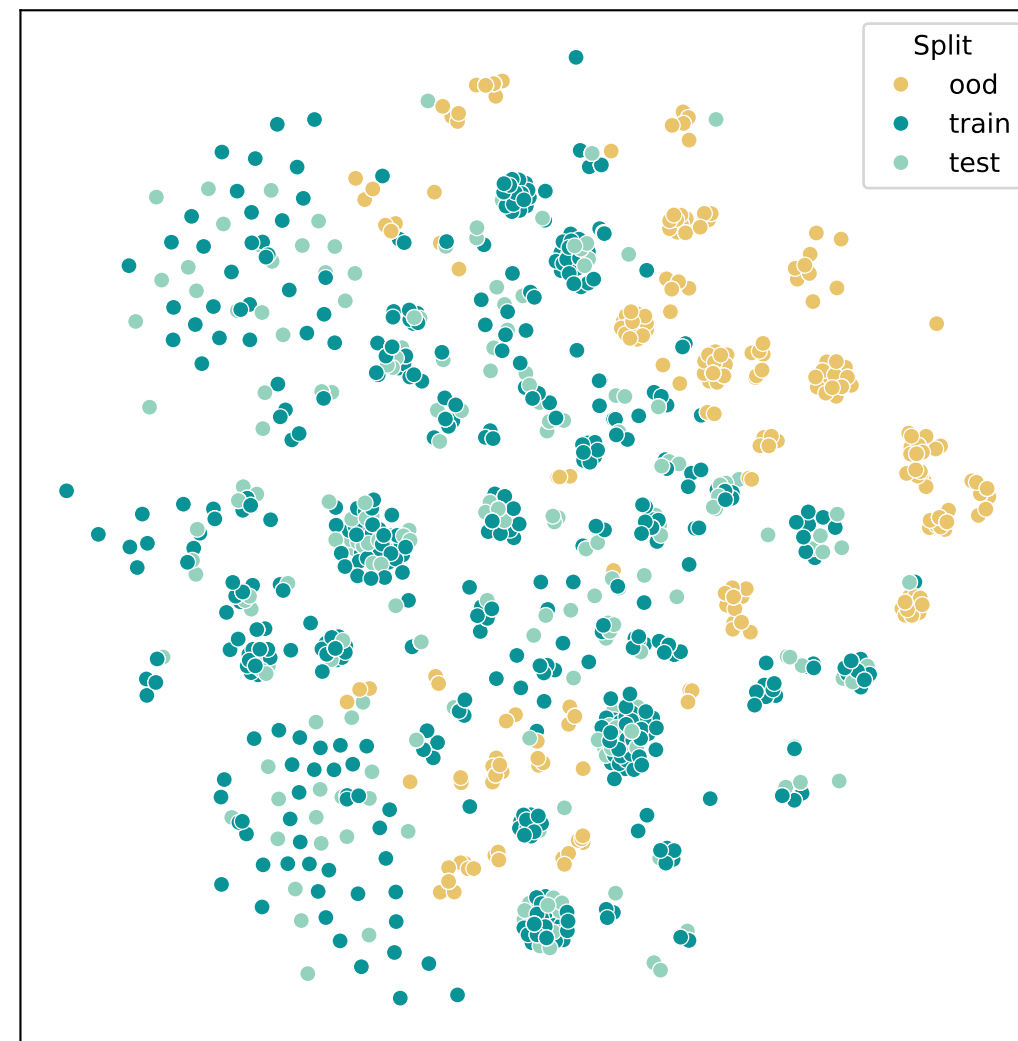


TSNE of CHEMBL235_EC50 (n=2303)



Whole molecule ECFPs



Cyclic skeleton ECFPs