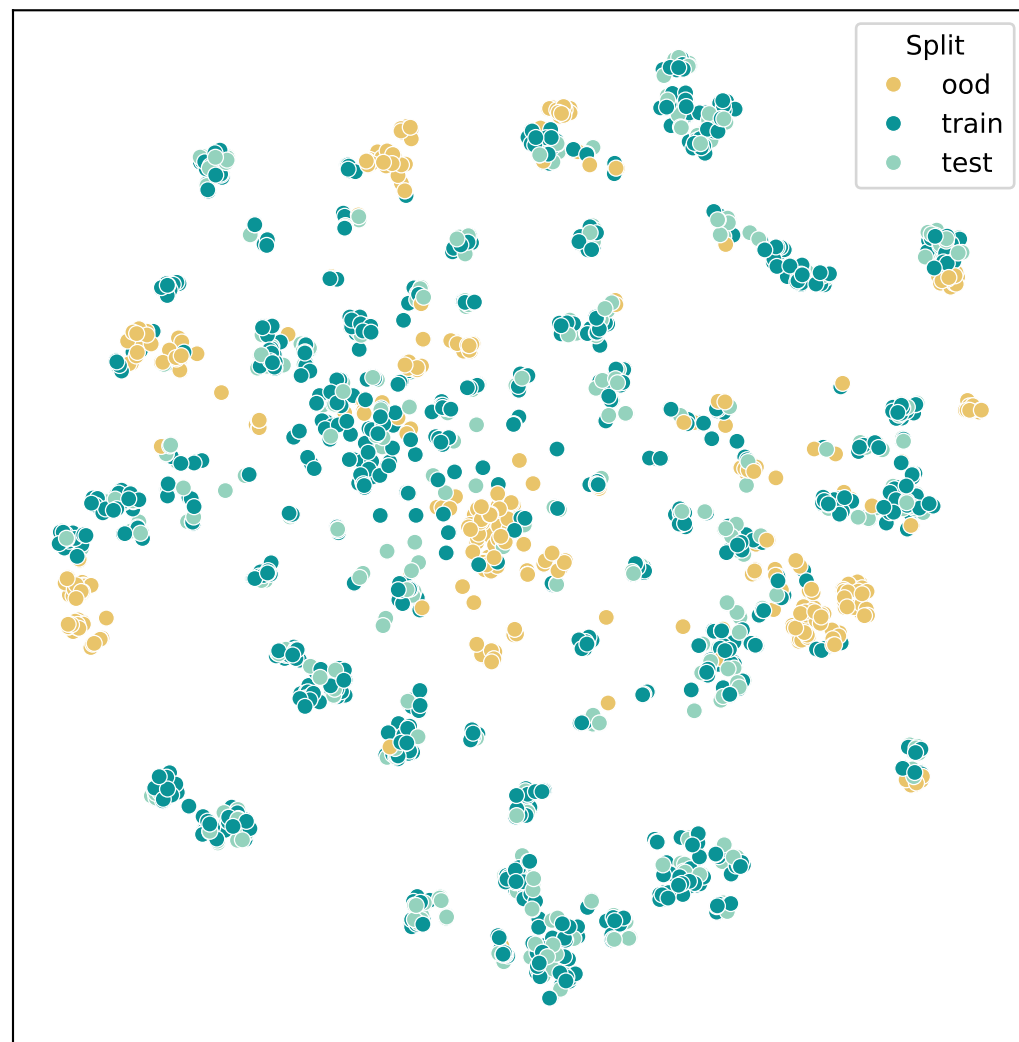
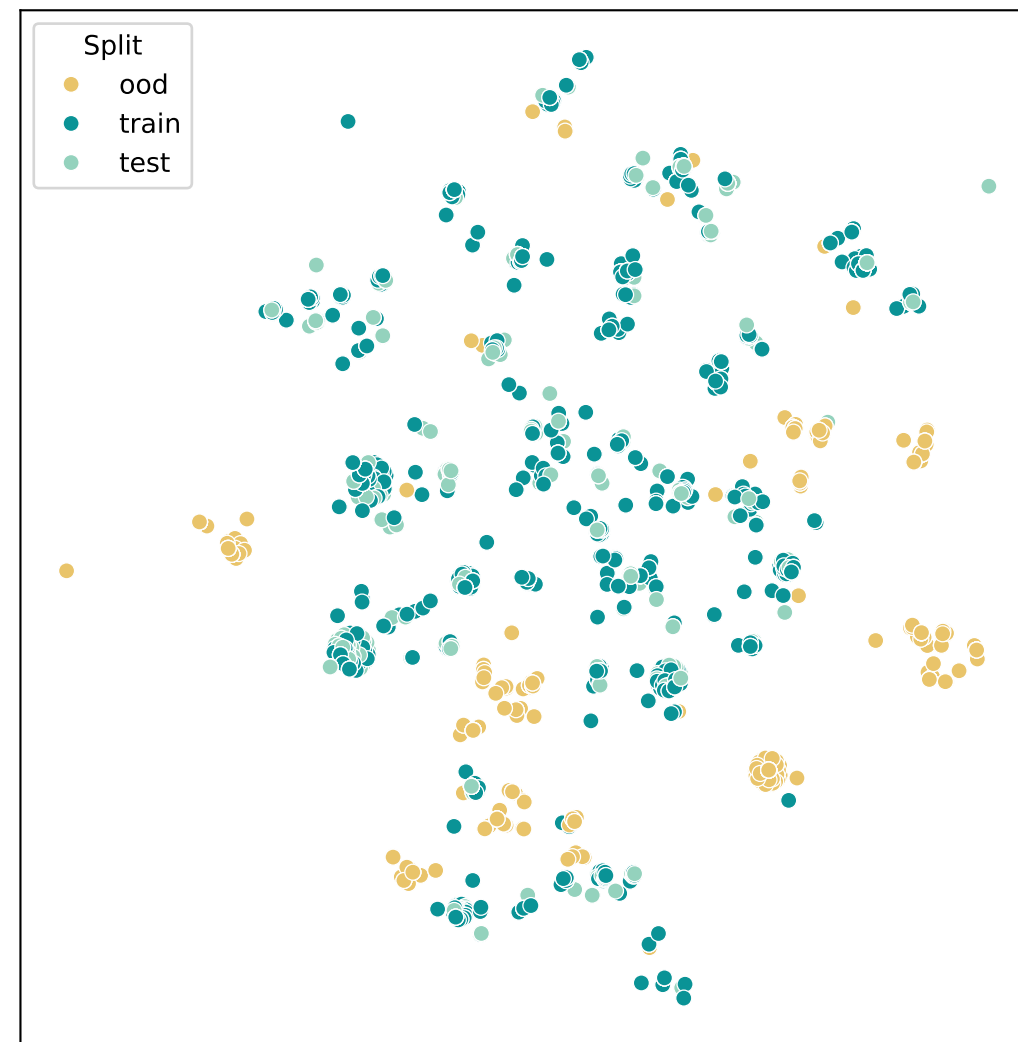


TSNE of CHEMBL204_Ki (n=2457)



Whole molecule ECFPs



Cyclic skeleton ECFPs