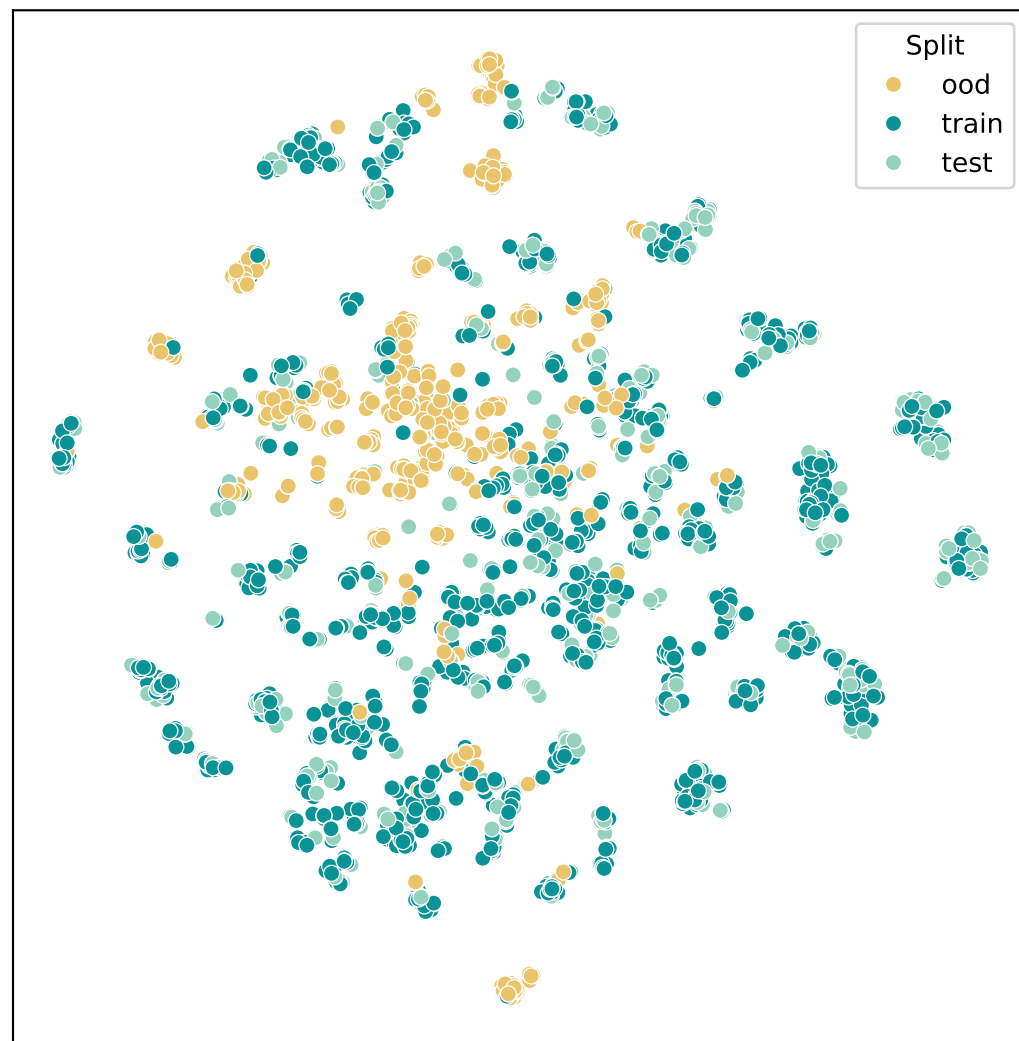
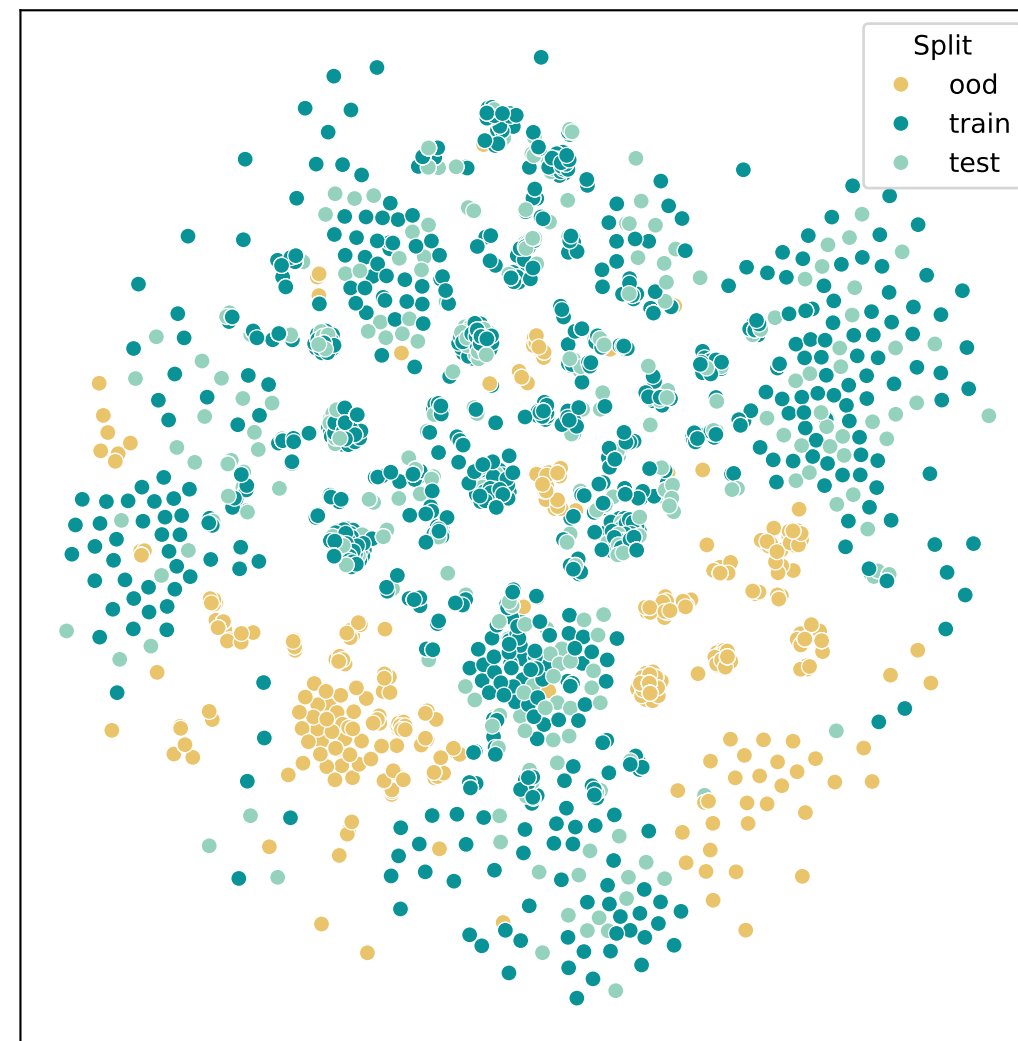


TSNE of CHEMBL234_Ki (n=3590)



Whole molecule ECFPs



Cyclic skeleton ECFPs