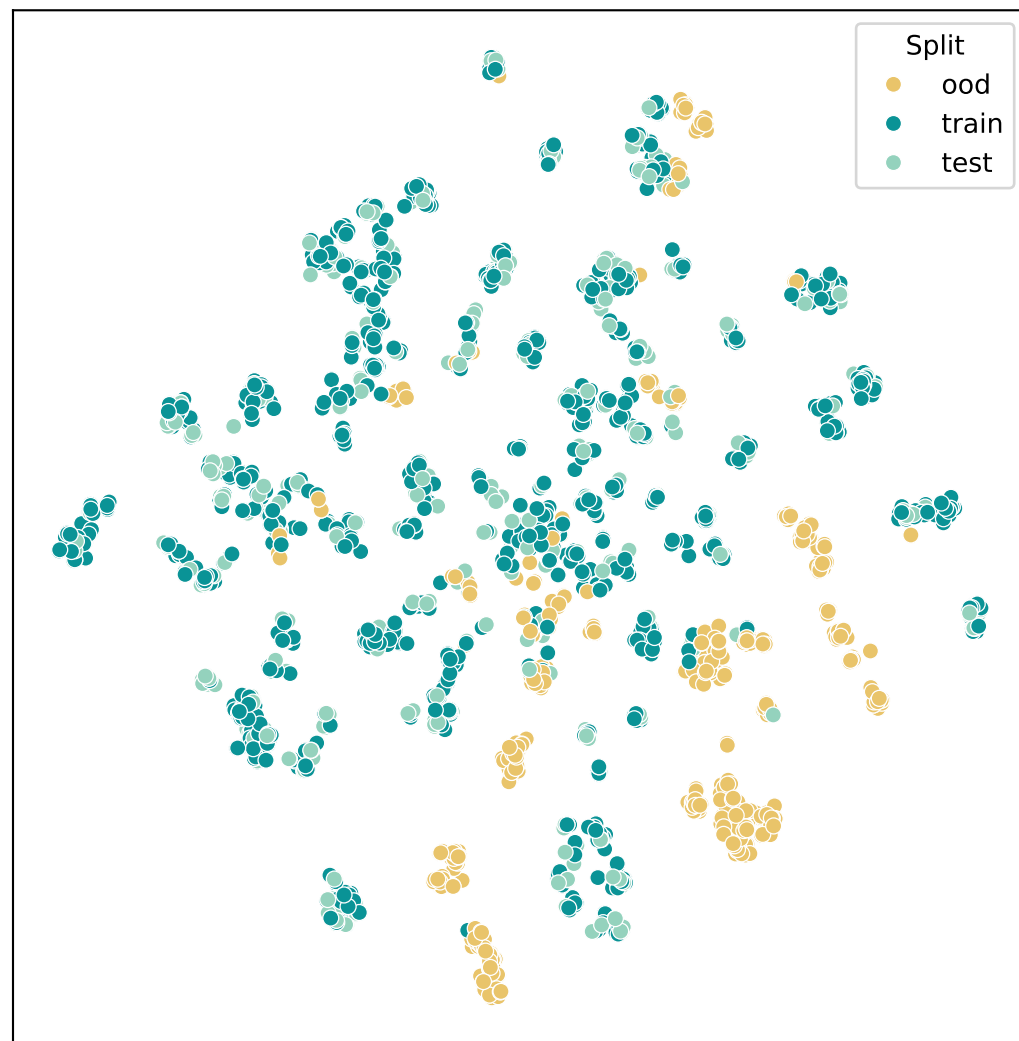
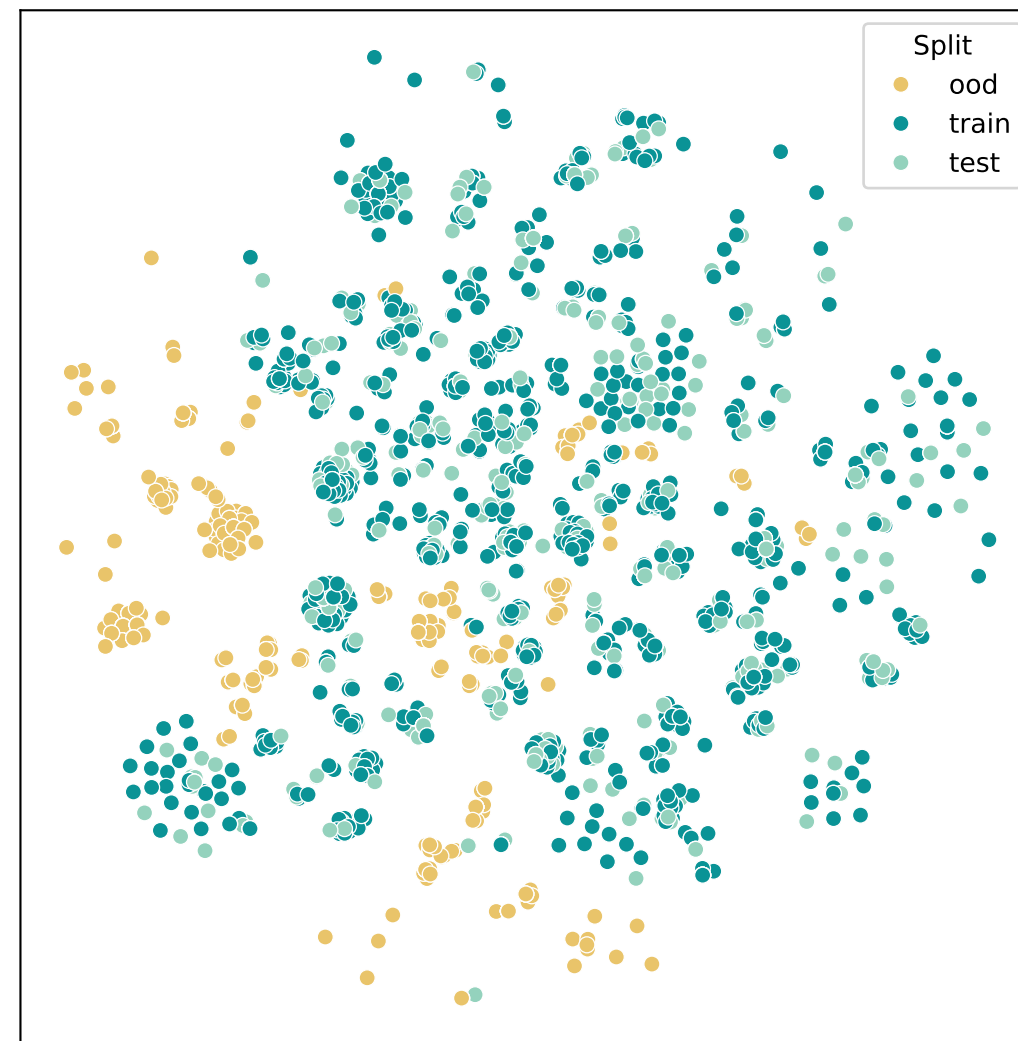


TSNE of CHEMBL233_Ki (n=2962)



Whole molecule ECFPs



Cyclic skeleton ECFPs