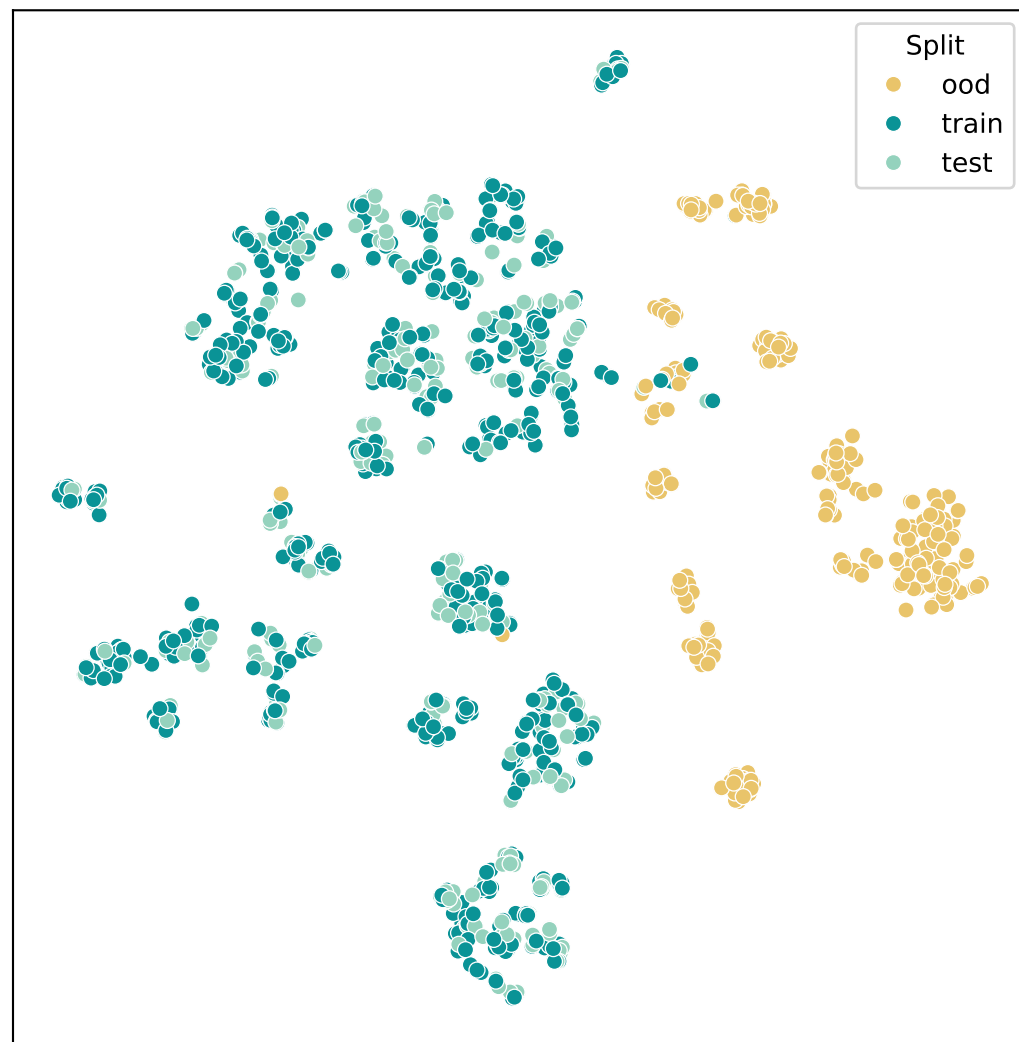
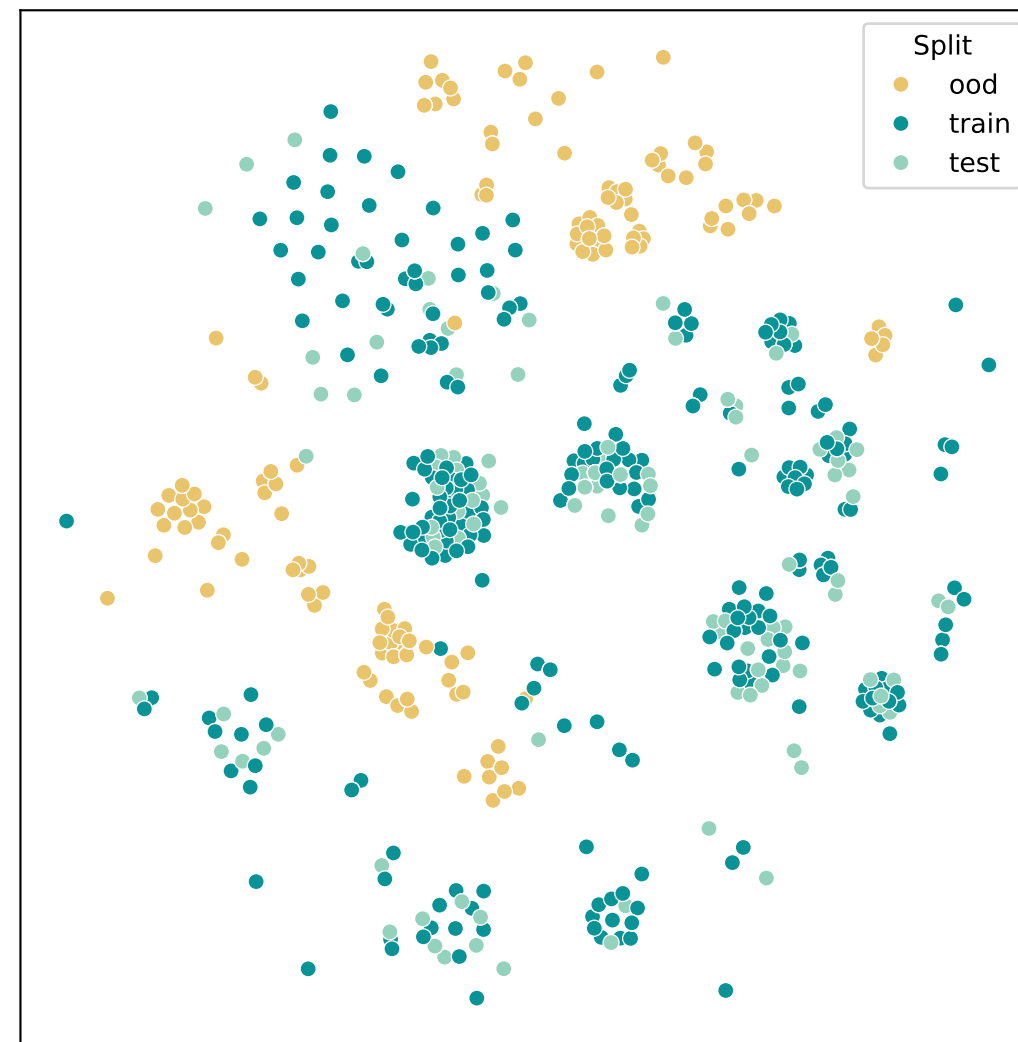


TSNE of ChEMBL4792\_Ki (n=1467)



Whole molecule ECFPs



Cyclic skeleton ECFPs