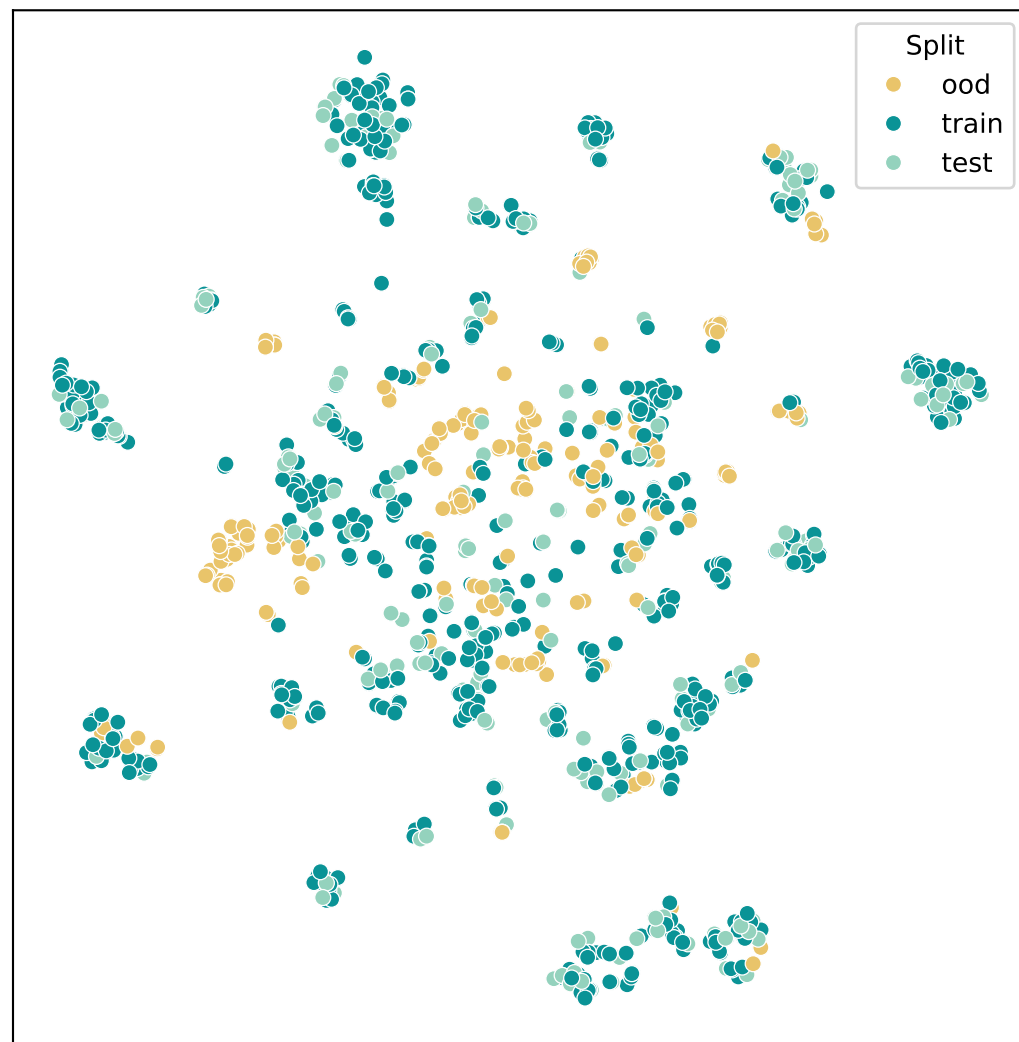
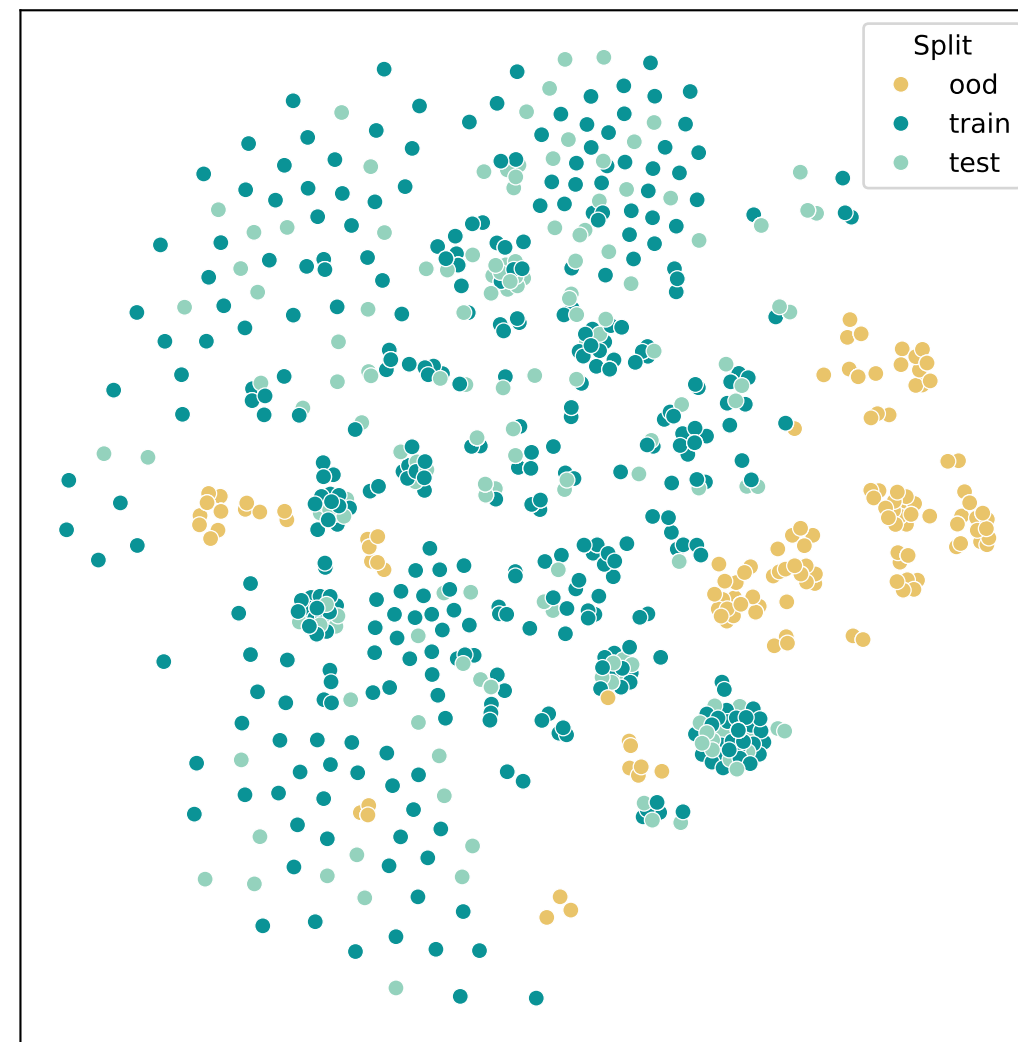


TSNE of ChEMBL287_Ki (n=1297)



Whole molecule ECFPs



Cyclic skeleton ECFPs