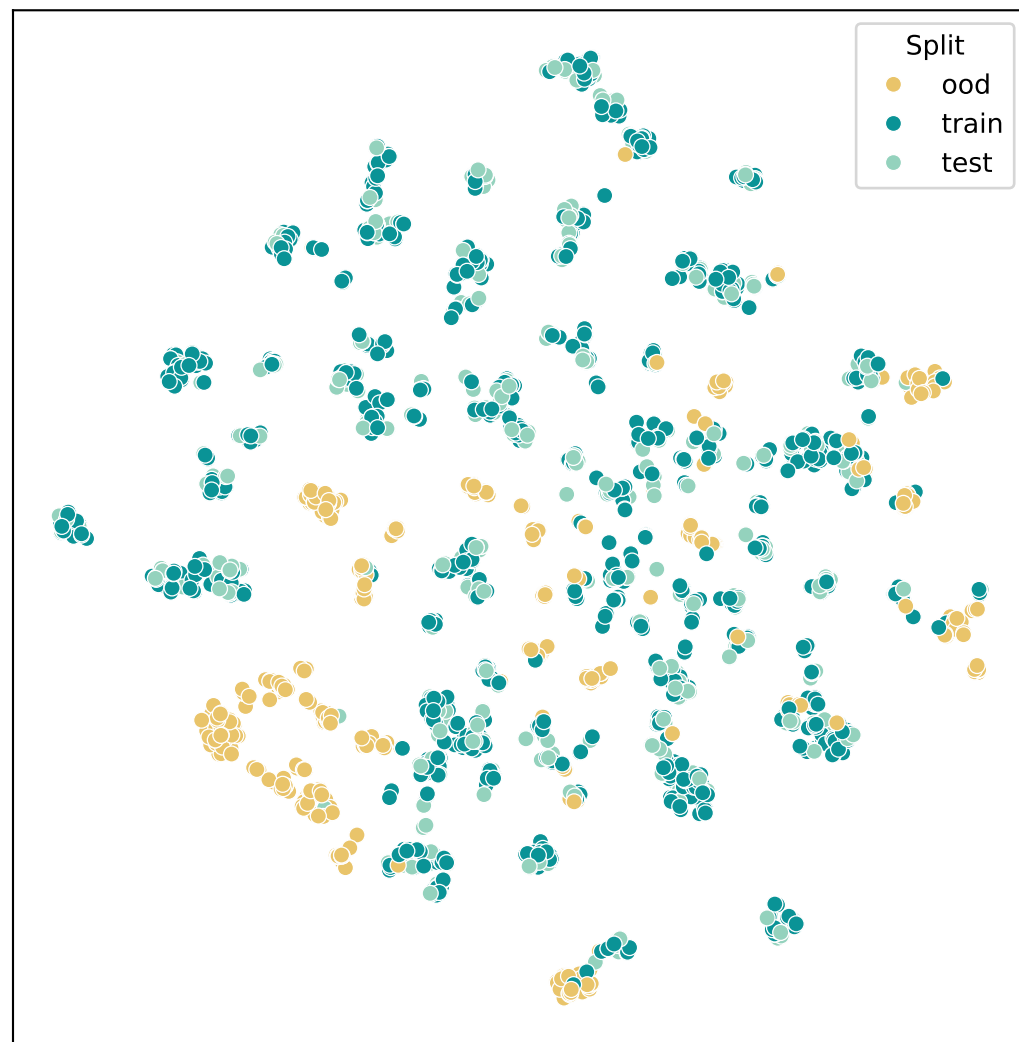
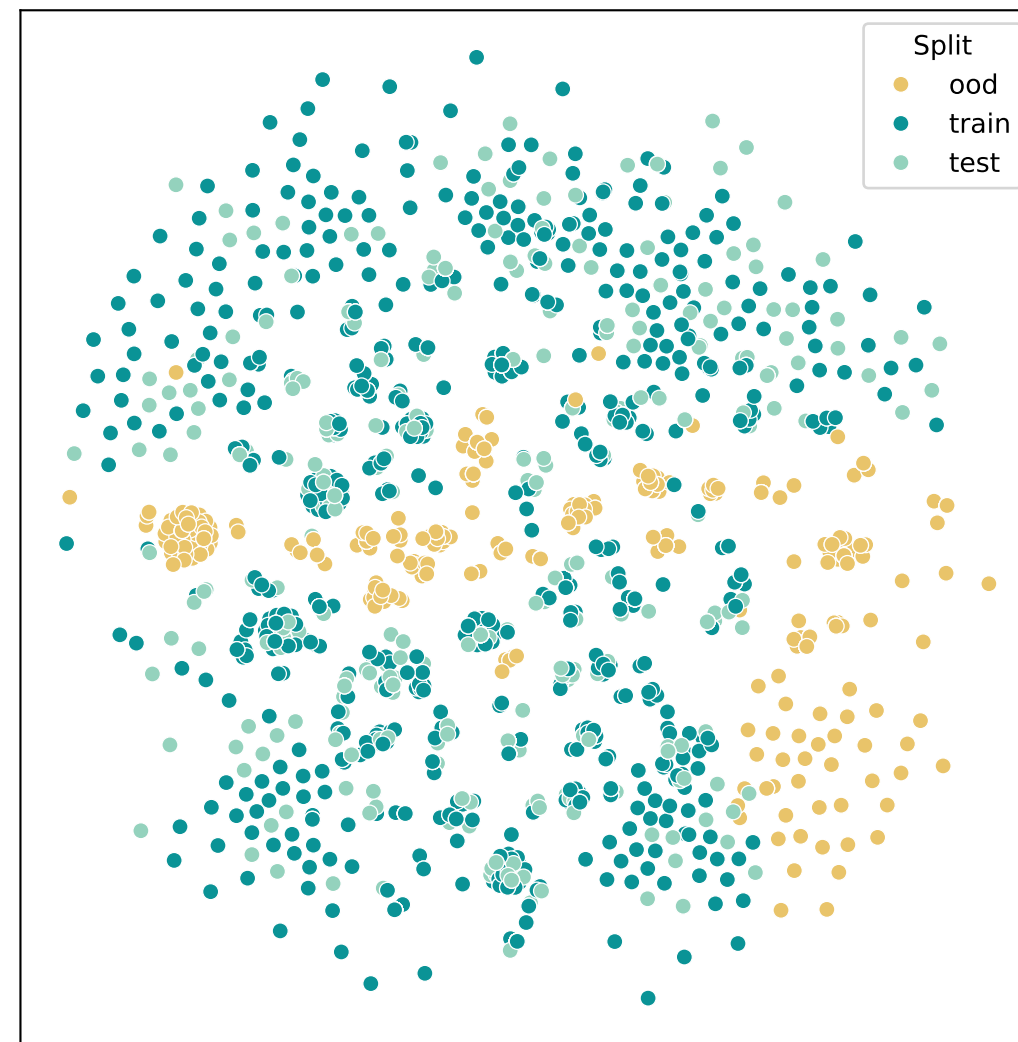


TSNE of CHEMBL244_Ki (n=2947)



Whole molecule ECFPs



Cyclic skeleton ECFPs