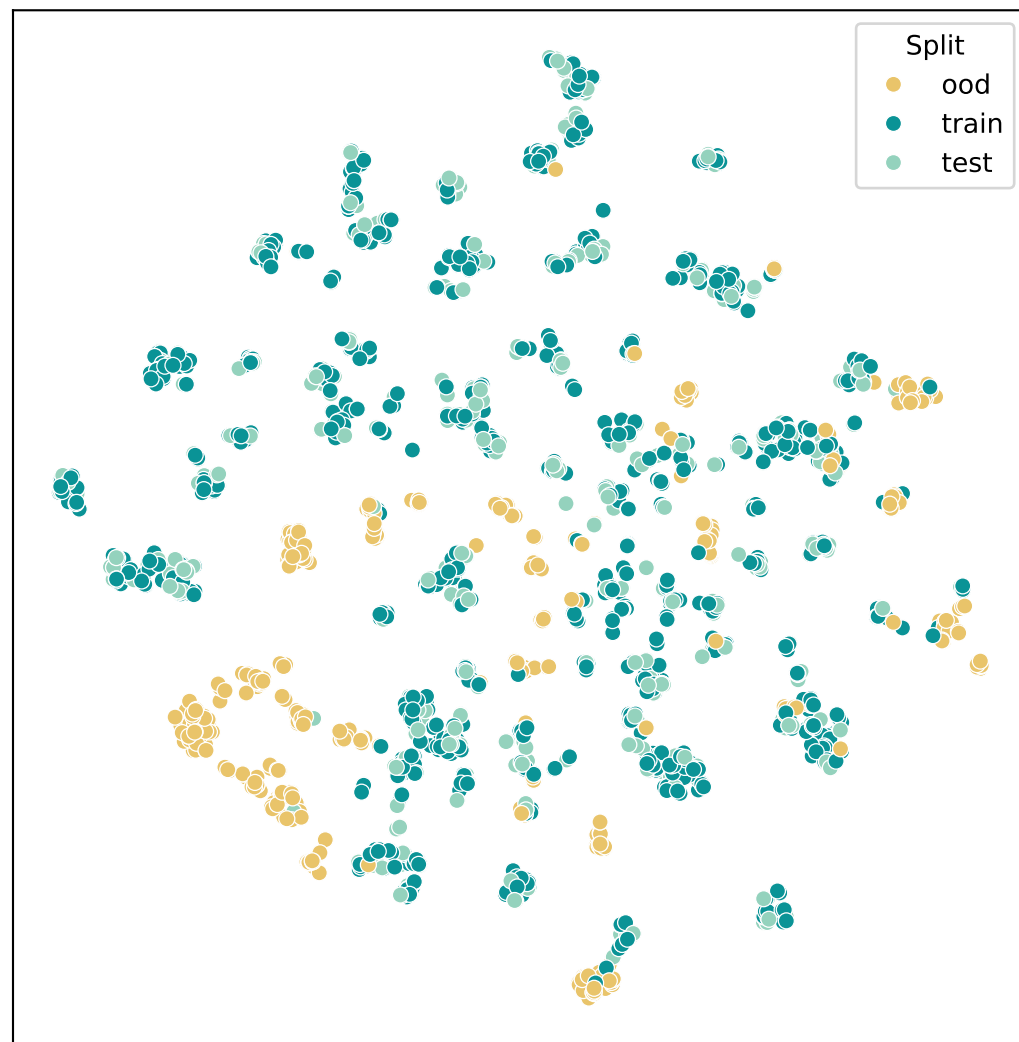
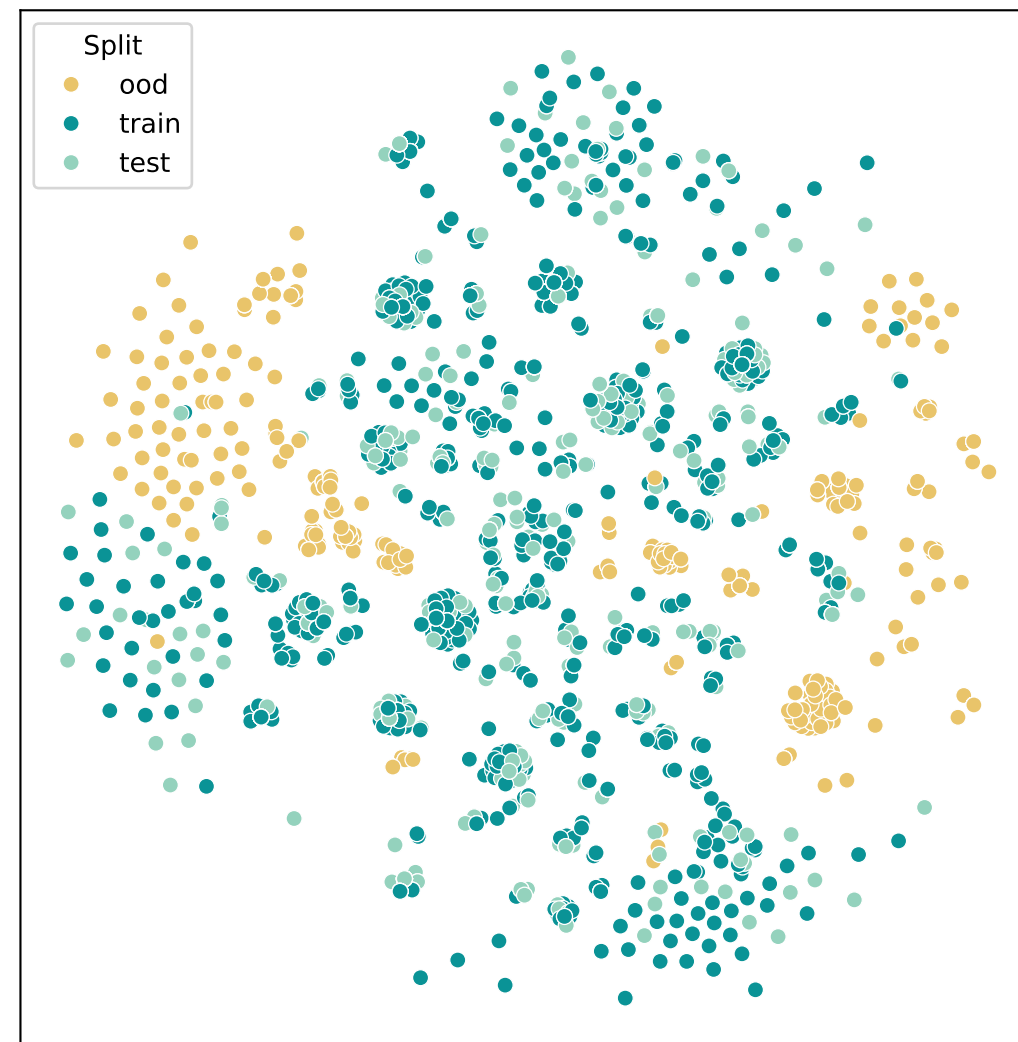


TSNE of CHEMBL244\_Ki (n=2947)



Whole molecule ECFPs



Cyclic skeleton ECFPs