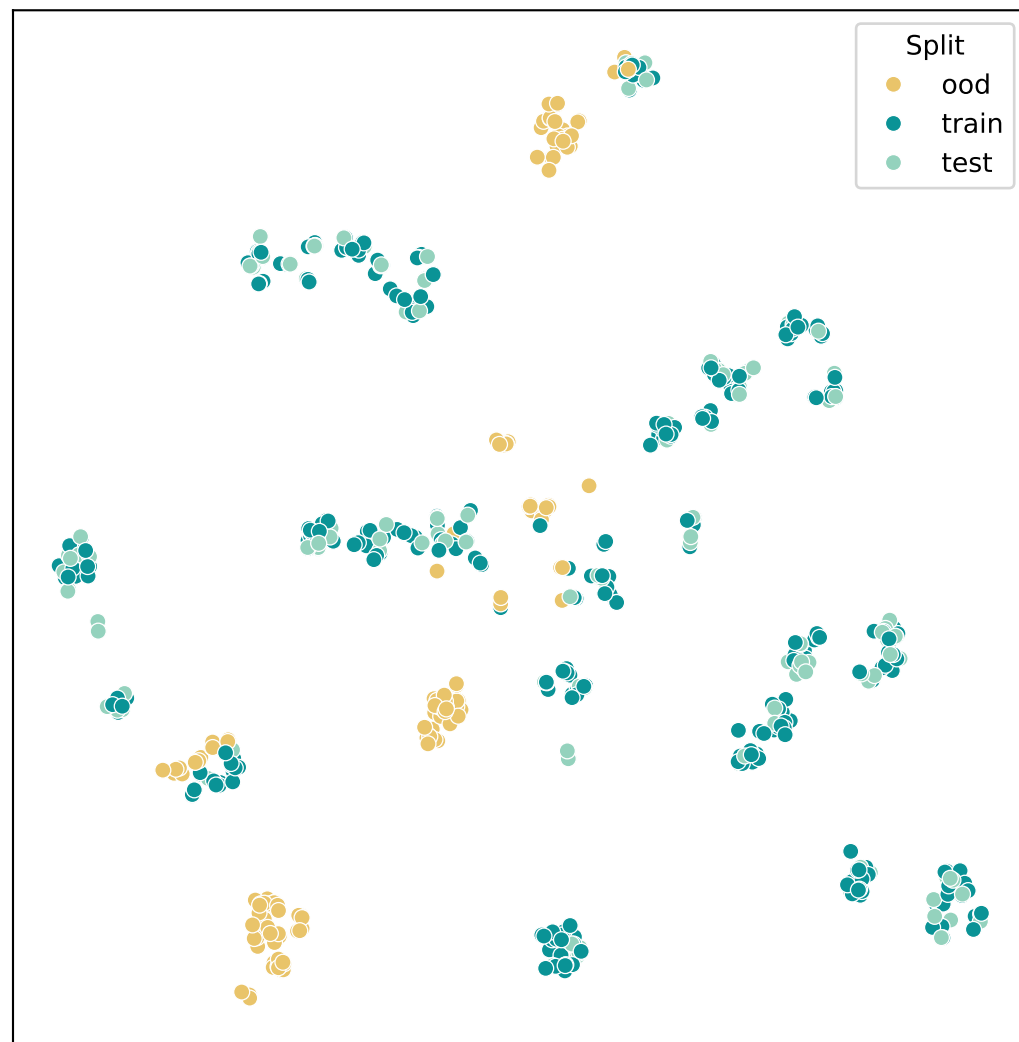
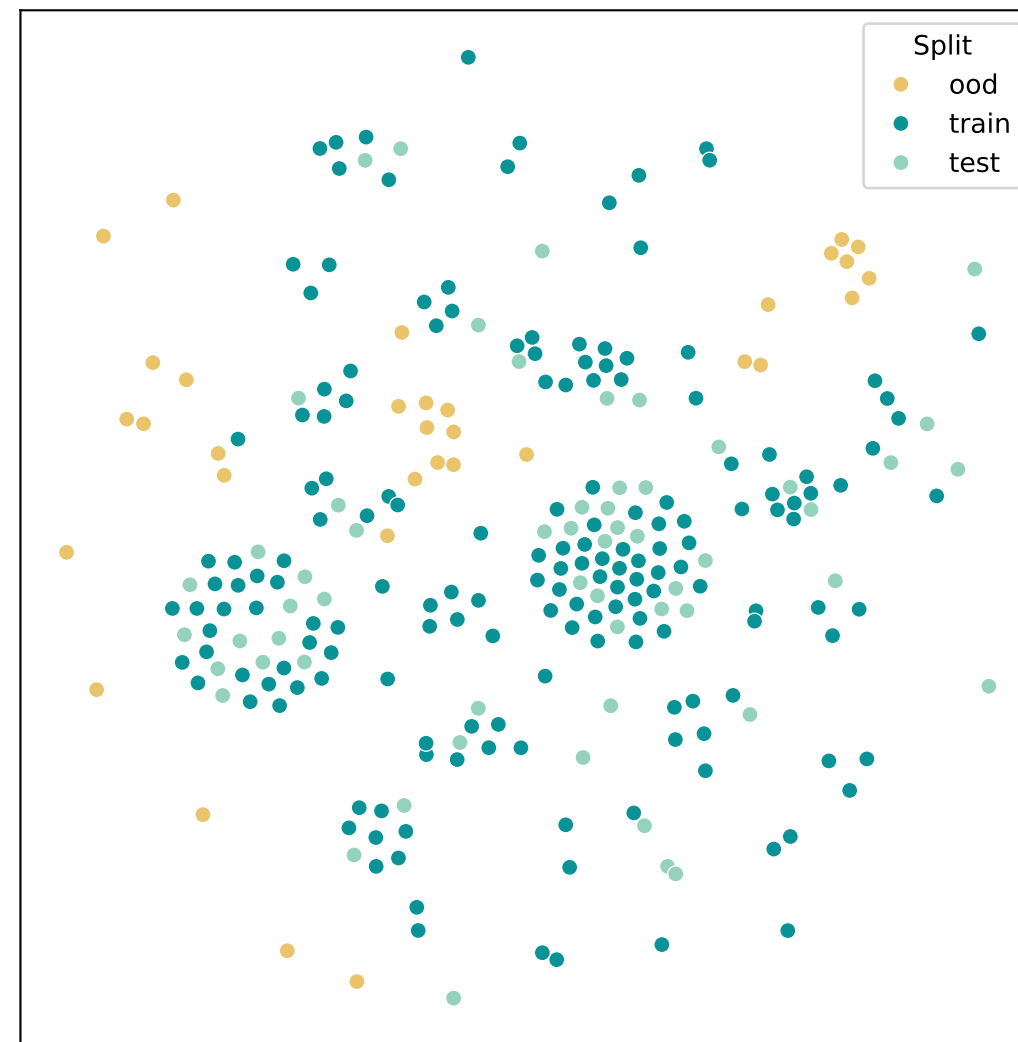


TSNE of CHEMBL2034\_Ki (n=726)



Whole molecule ECFPs



Cyclic skeleton ECFPs