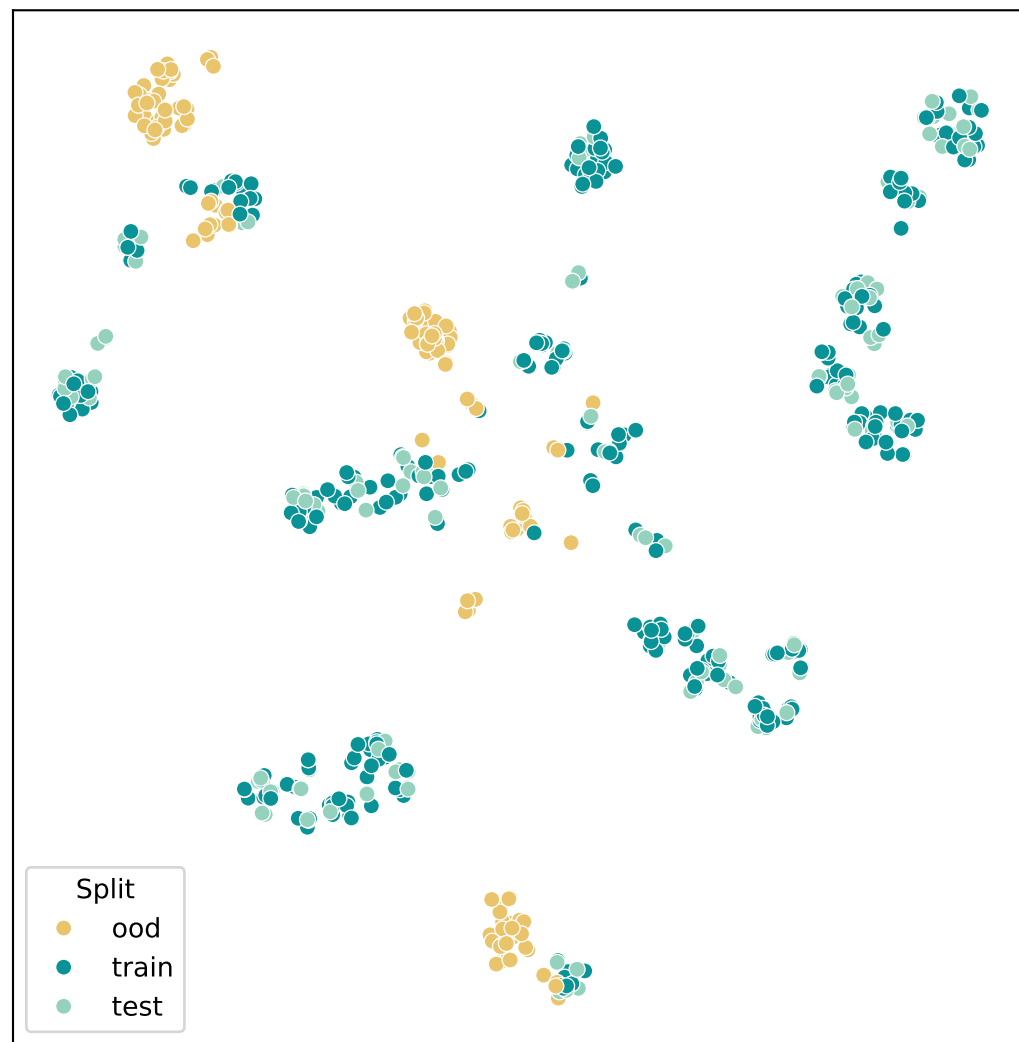
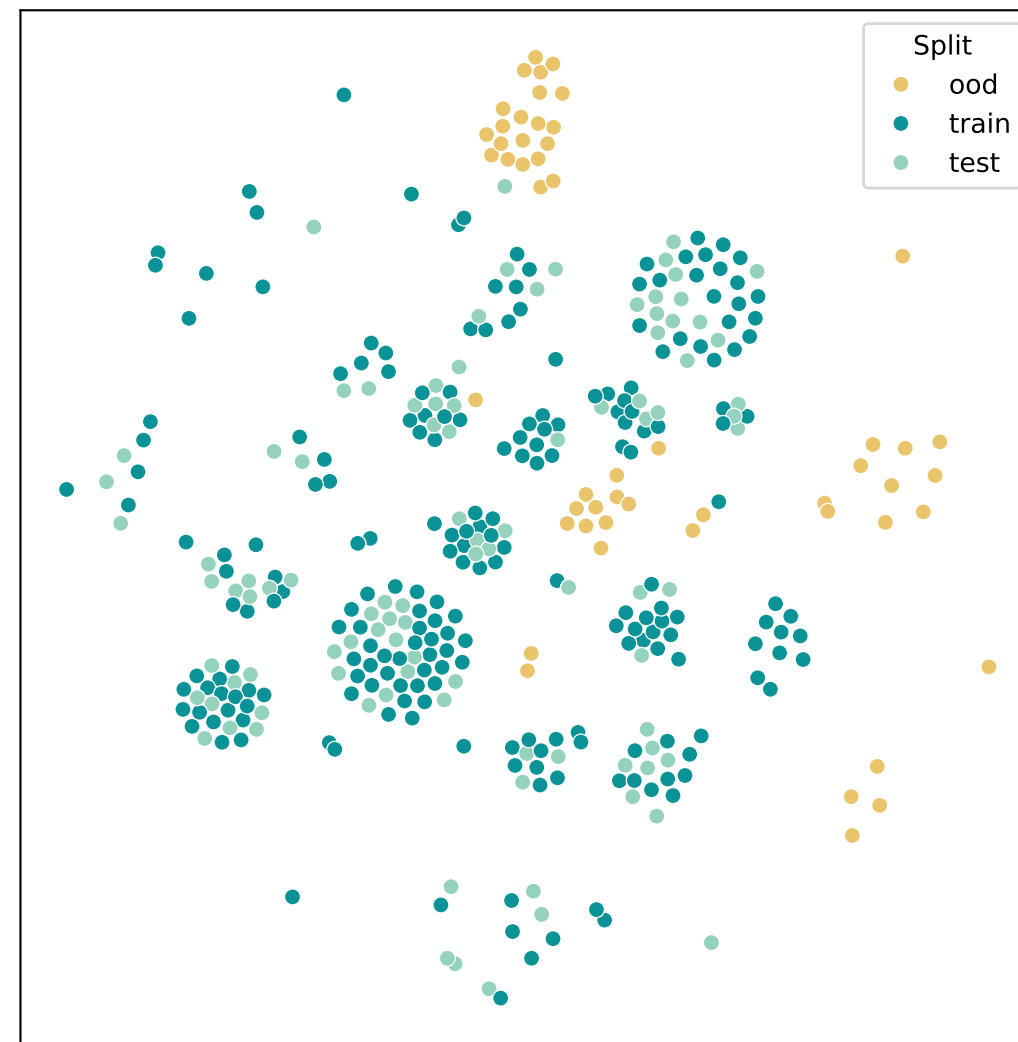


TSNE of CHEMBL2034_Ki (n=726)



Whole molecule ECFPs



Cyclic skeleton ECFPs