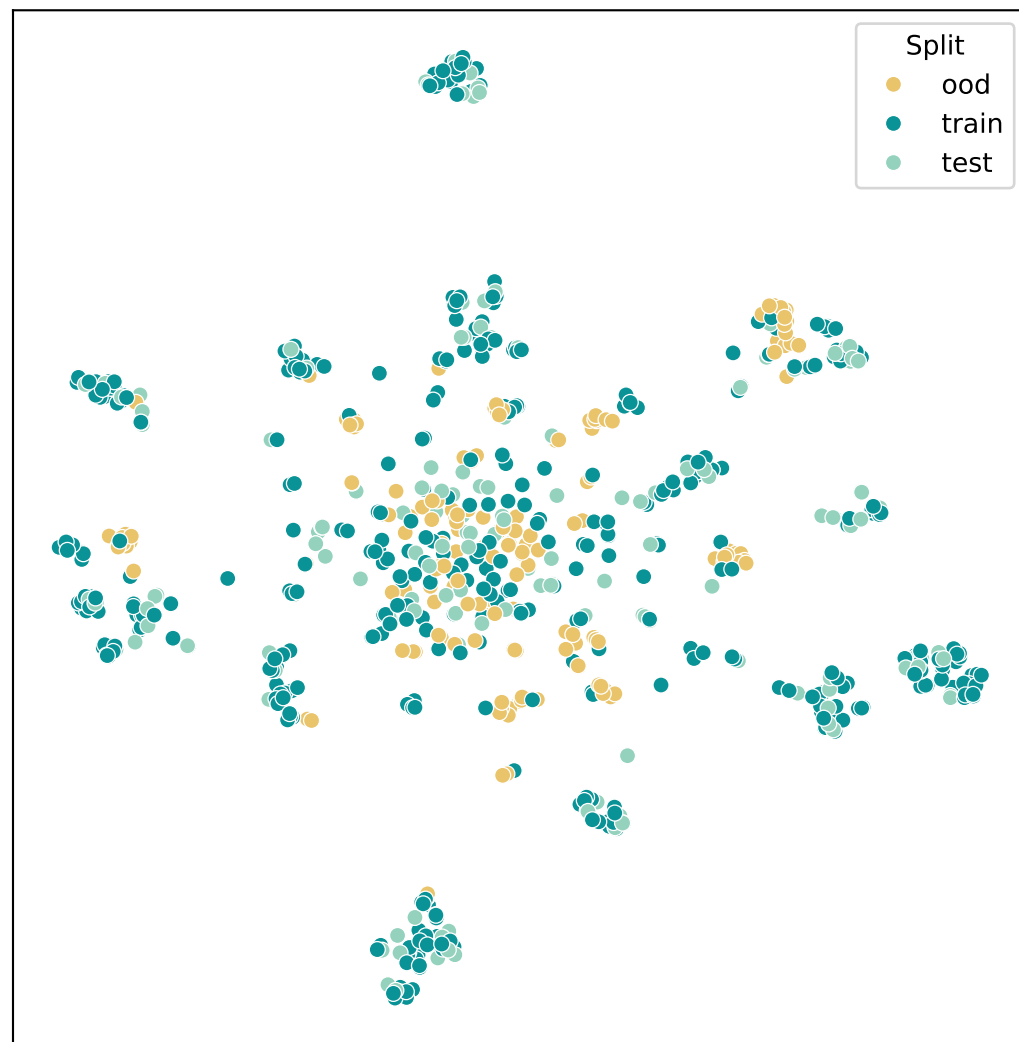
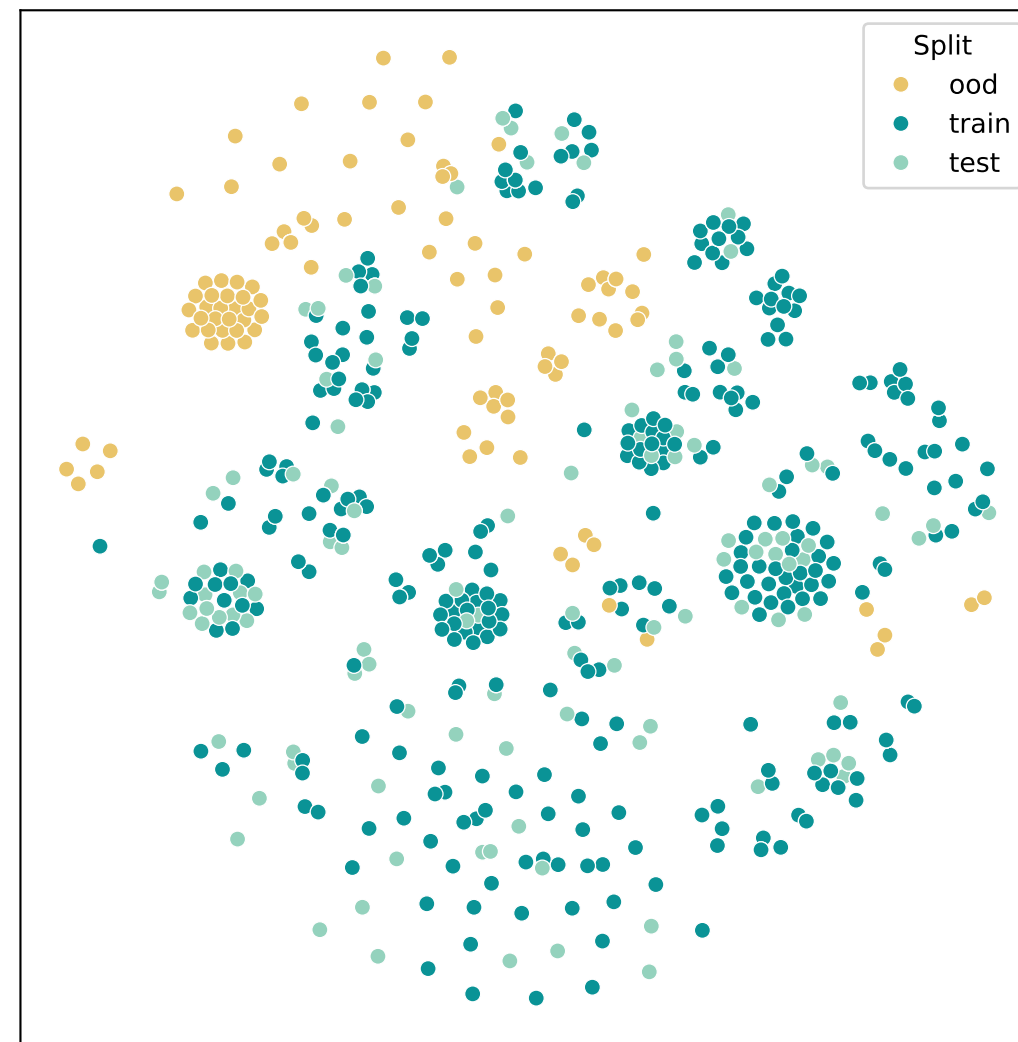


TSNE of CHEMBL262_Ki (n=835)



Whole molecule ECFPs



Cyclic skeleton ECFPs