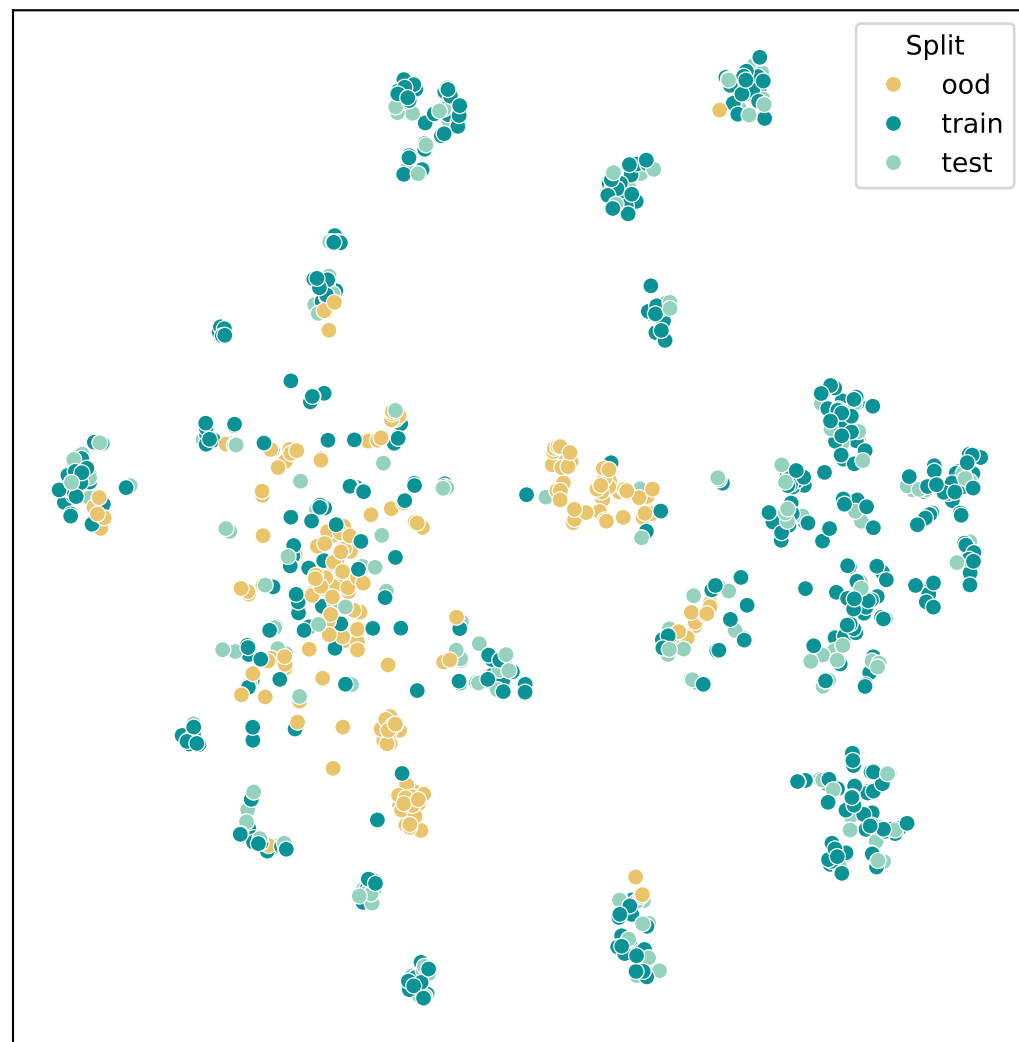
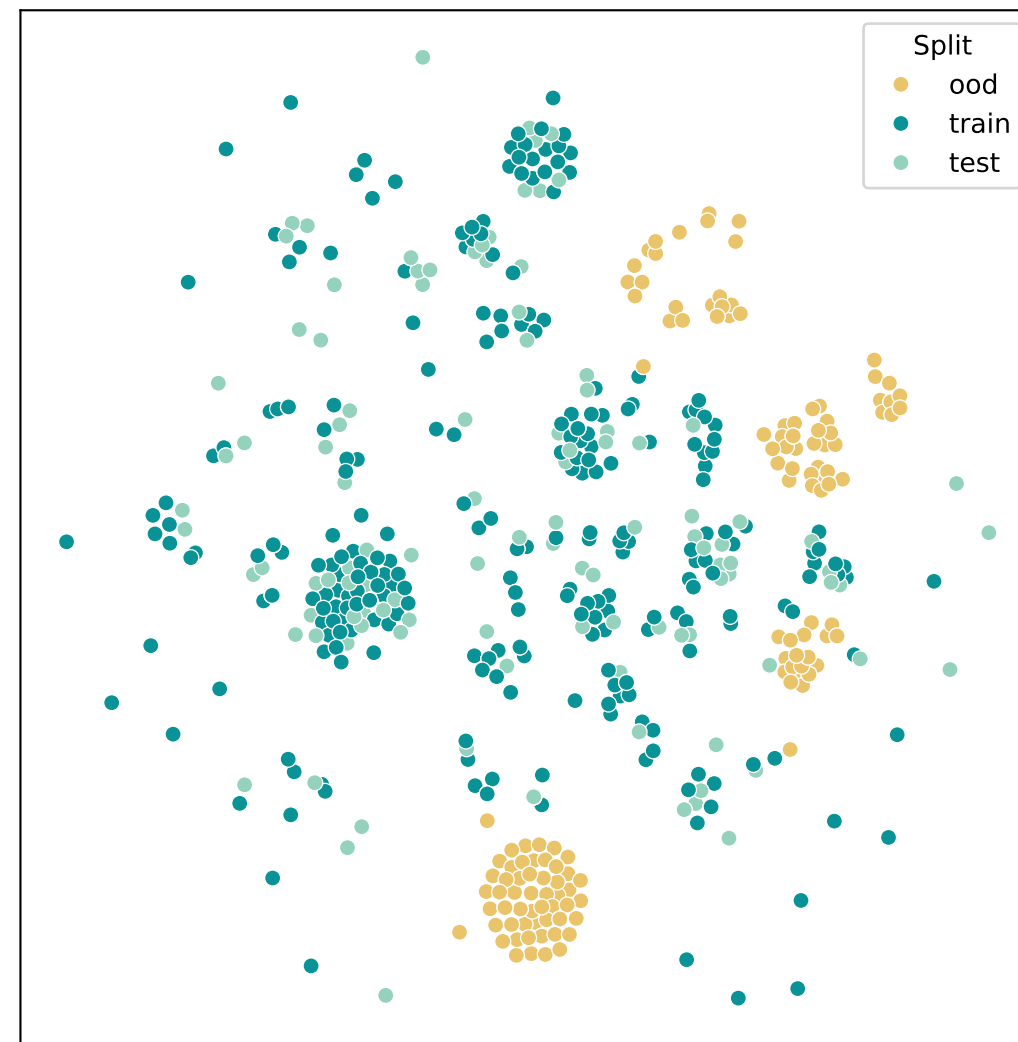


TSNE of CHEMBL2971\_Ki (n=966)



Whole molecule ECFPs



Cyclic skeleton ECFPs