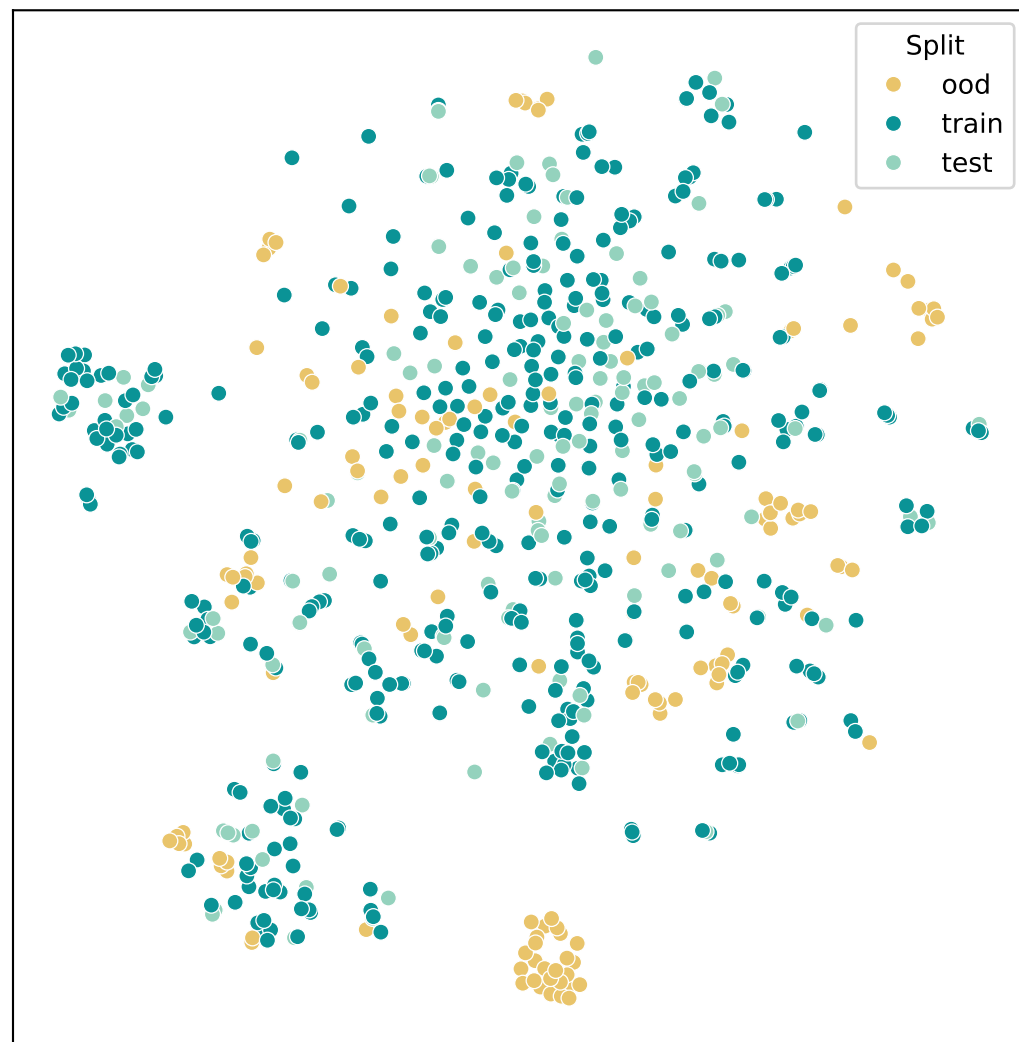
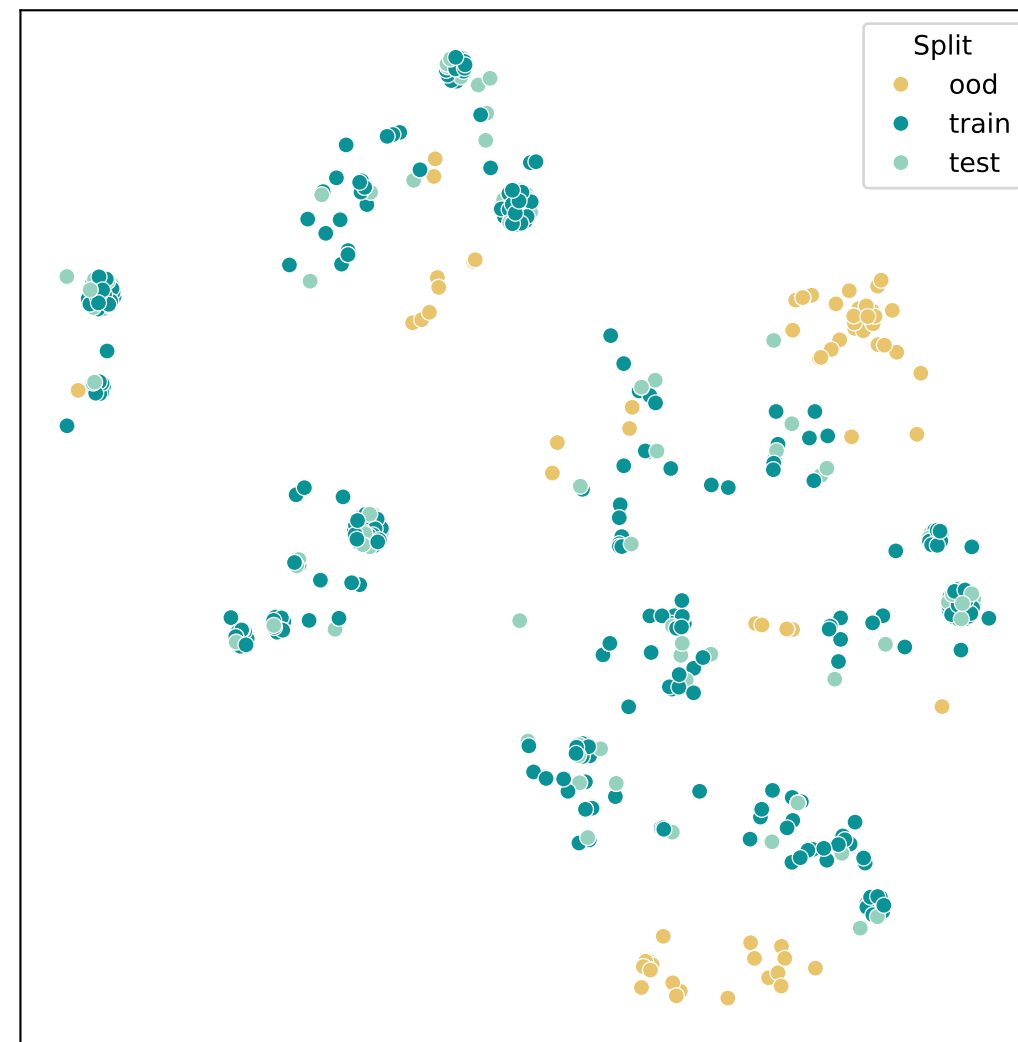


TSNE of CHEMBL4203\_Ki (n=717)



Whole molecule ECFPs



Cyclic skeleton ECFPs