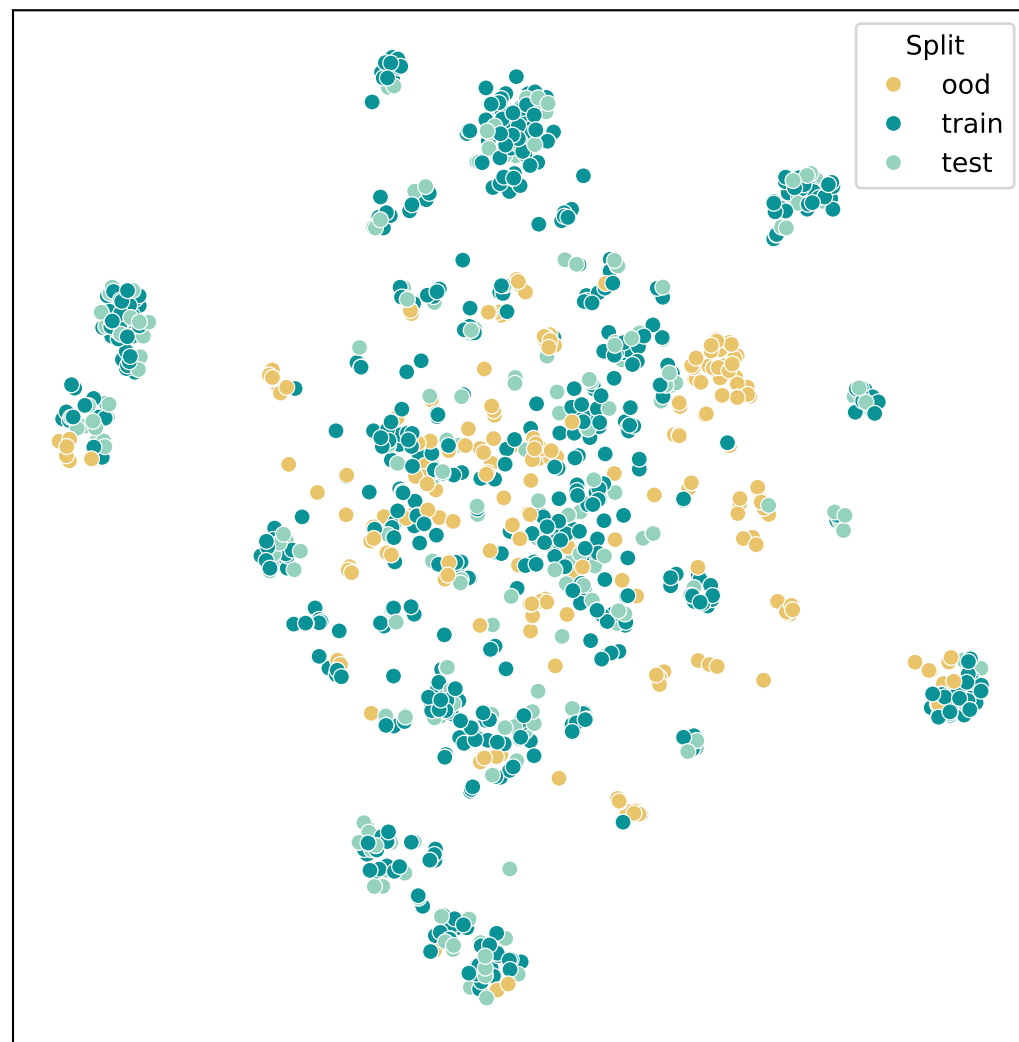
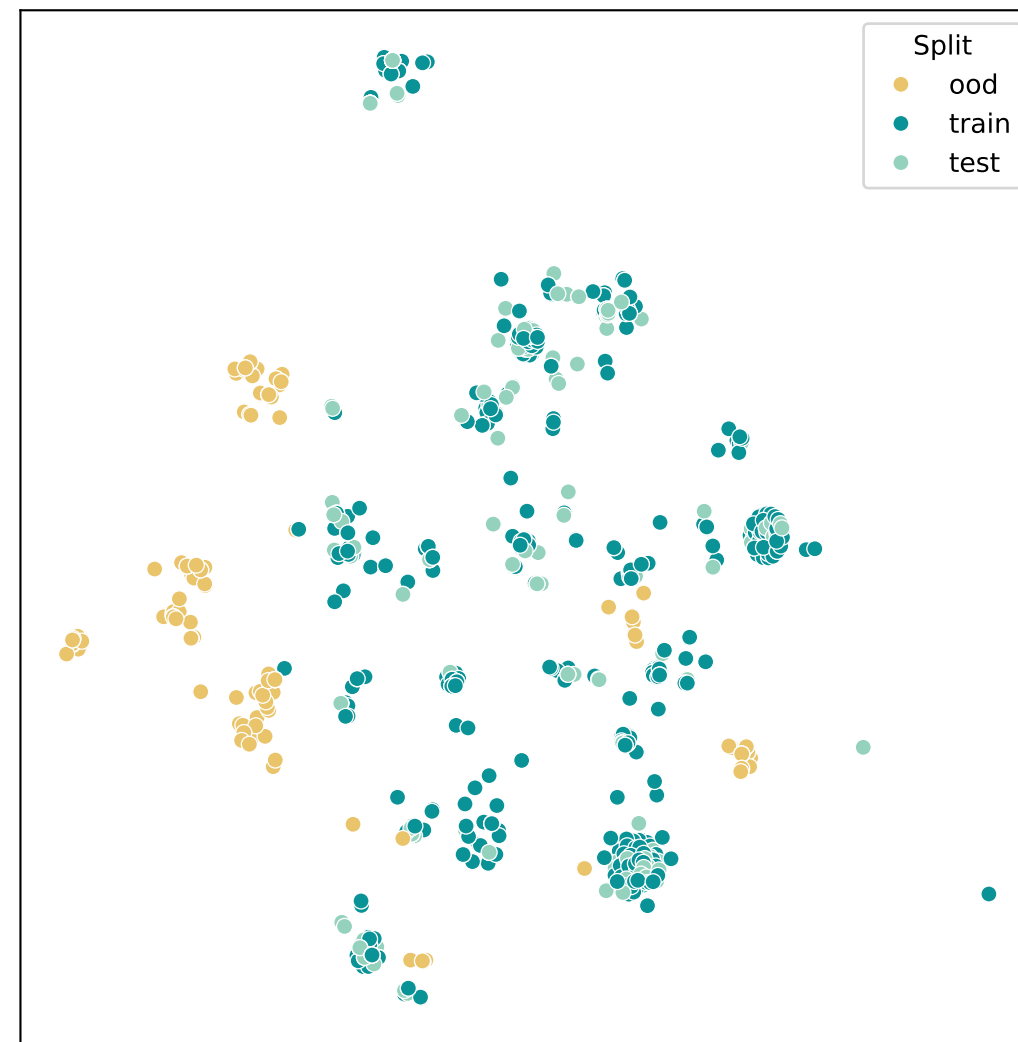


TSNE of CHEMBL287\_Ki (n=1297)



Whole molecule ECFPs



Cyclic skeleton ECFPs