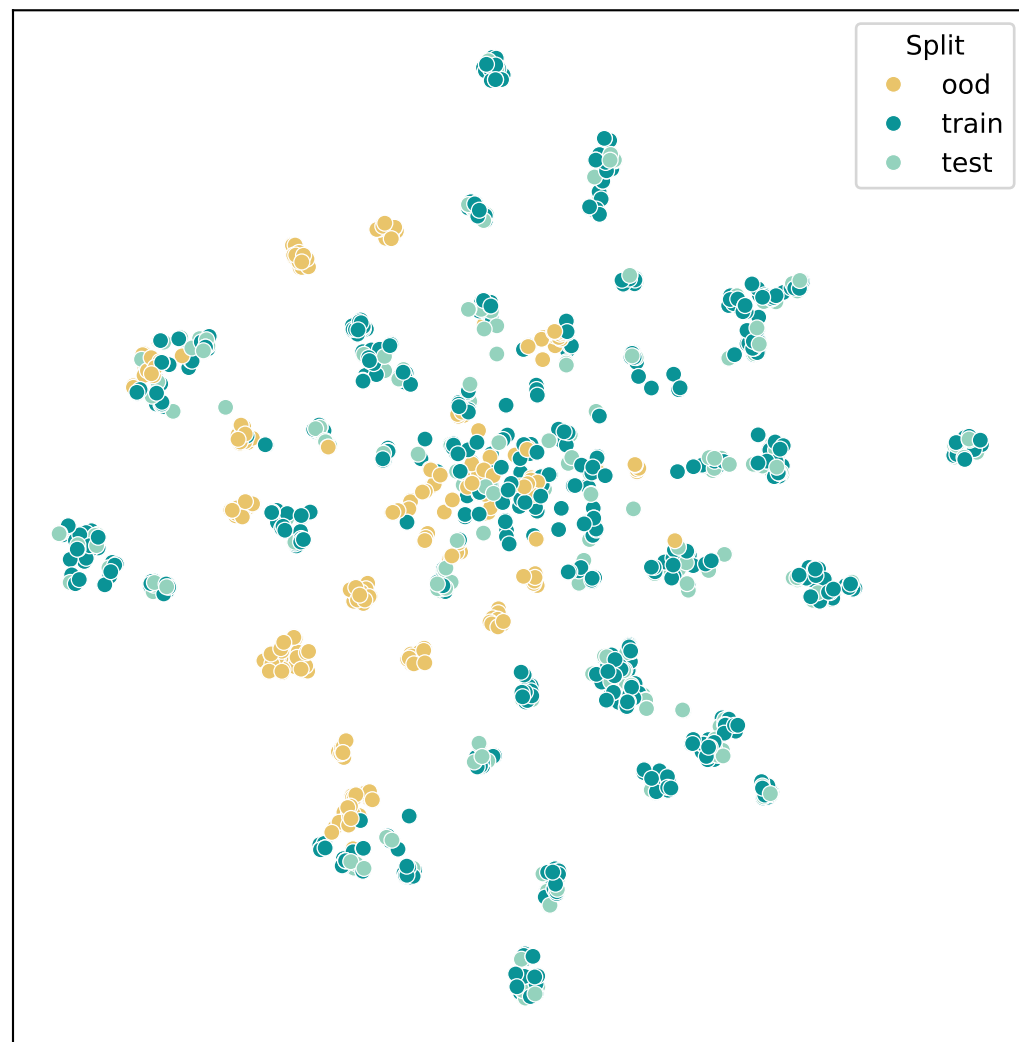
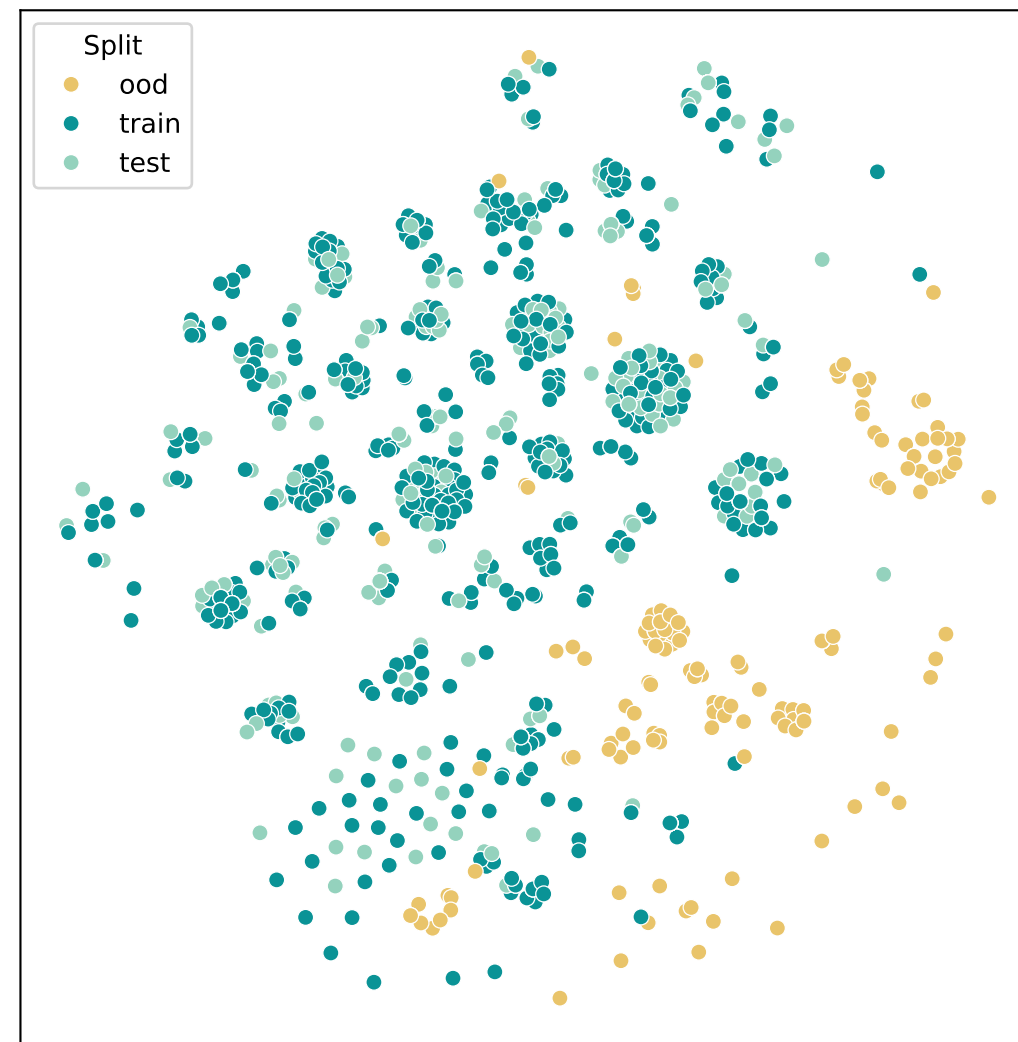


TSNE of CHEMBL228_Ki (n=1681)



Whole molecule ECFPs



Cyclic skeleton ECFPs