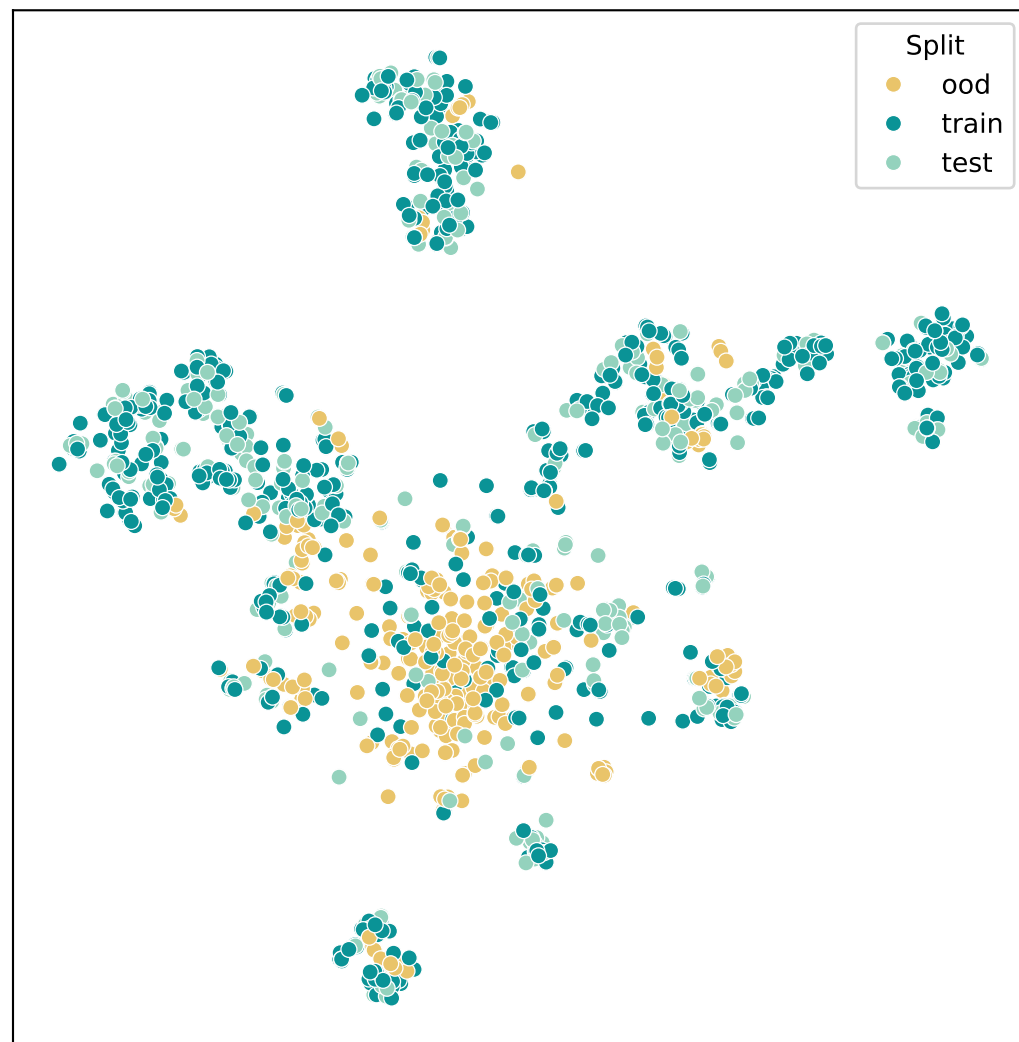
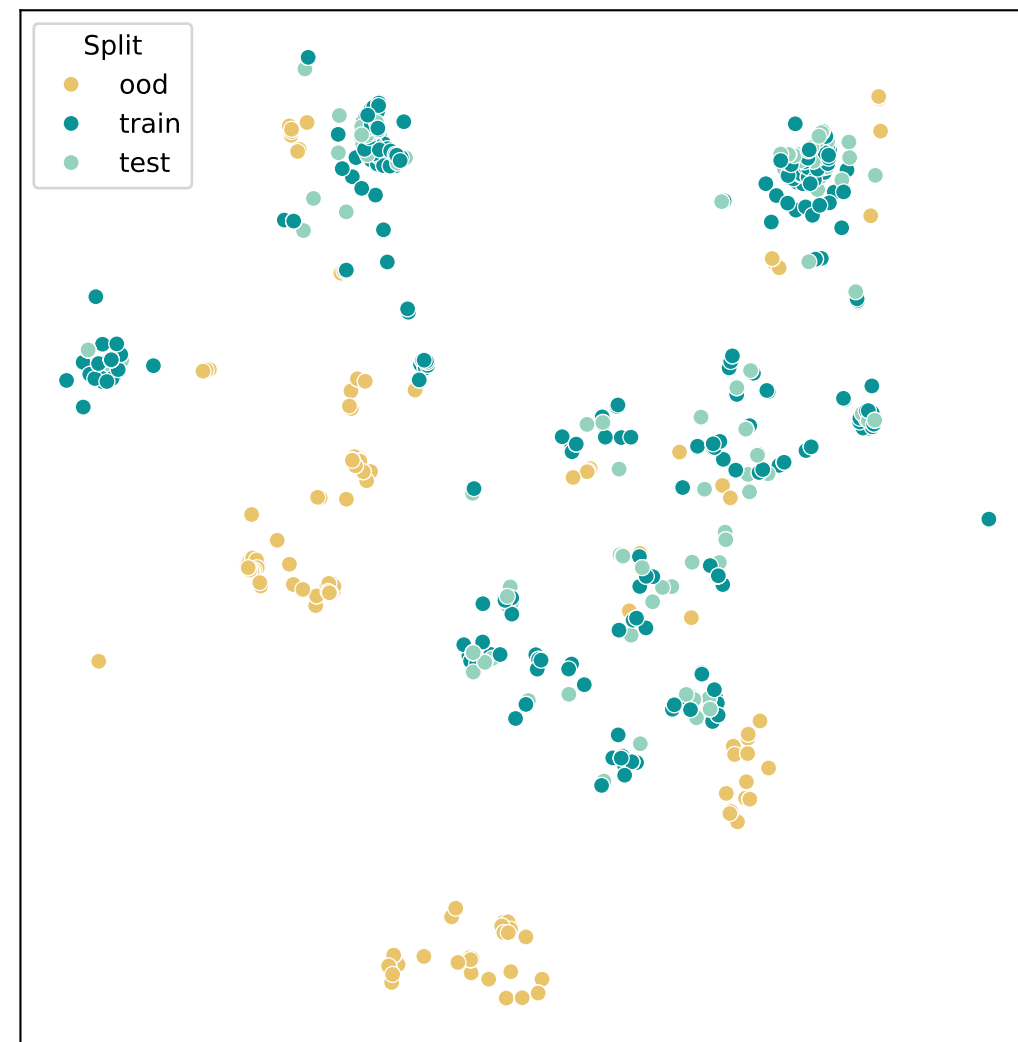


TSNE of CHEMBL2147_Ki (n=1443)



Whole molecule ECFPs



Cyclic skeleton ECFPs