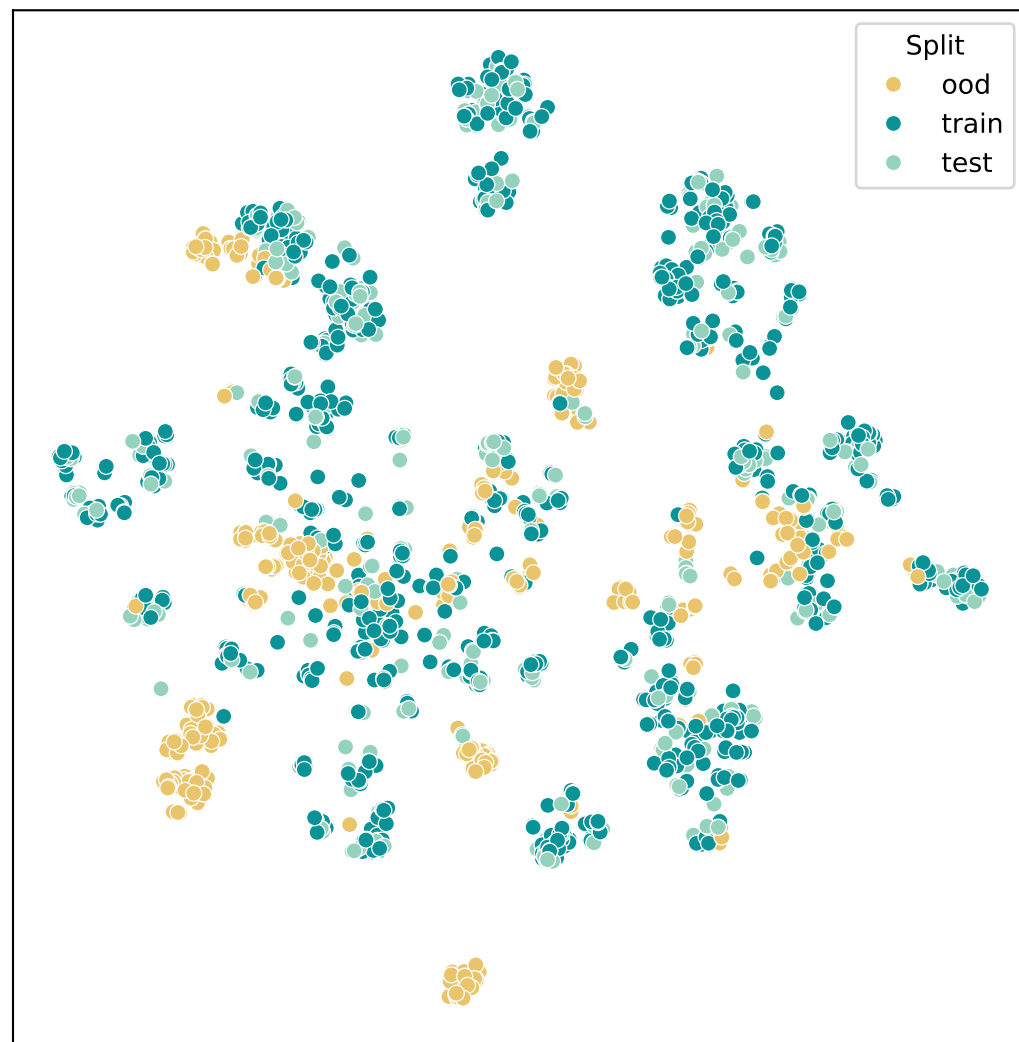
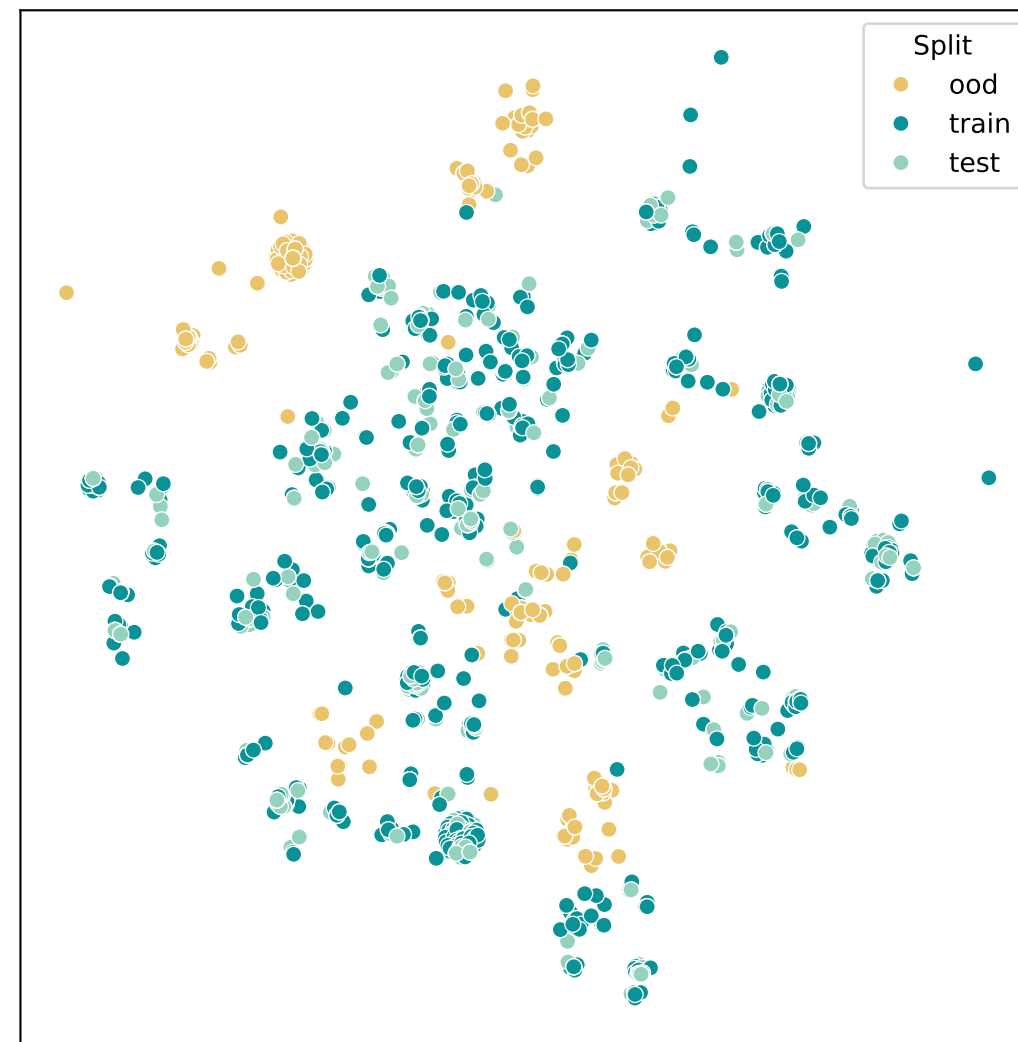


TSNE of CHEMBL237_Ki (n=2460)



Whole molecule ECFPs



Cyclic skeleton ECFPs