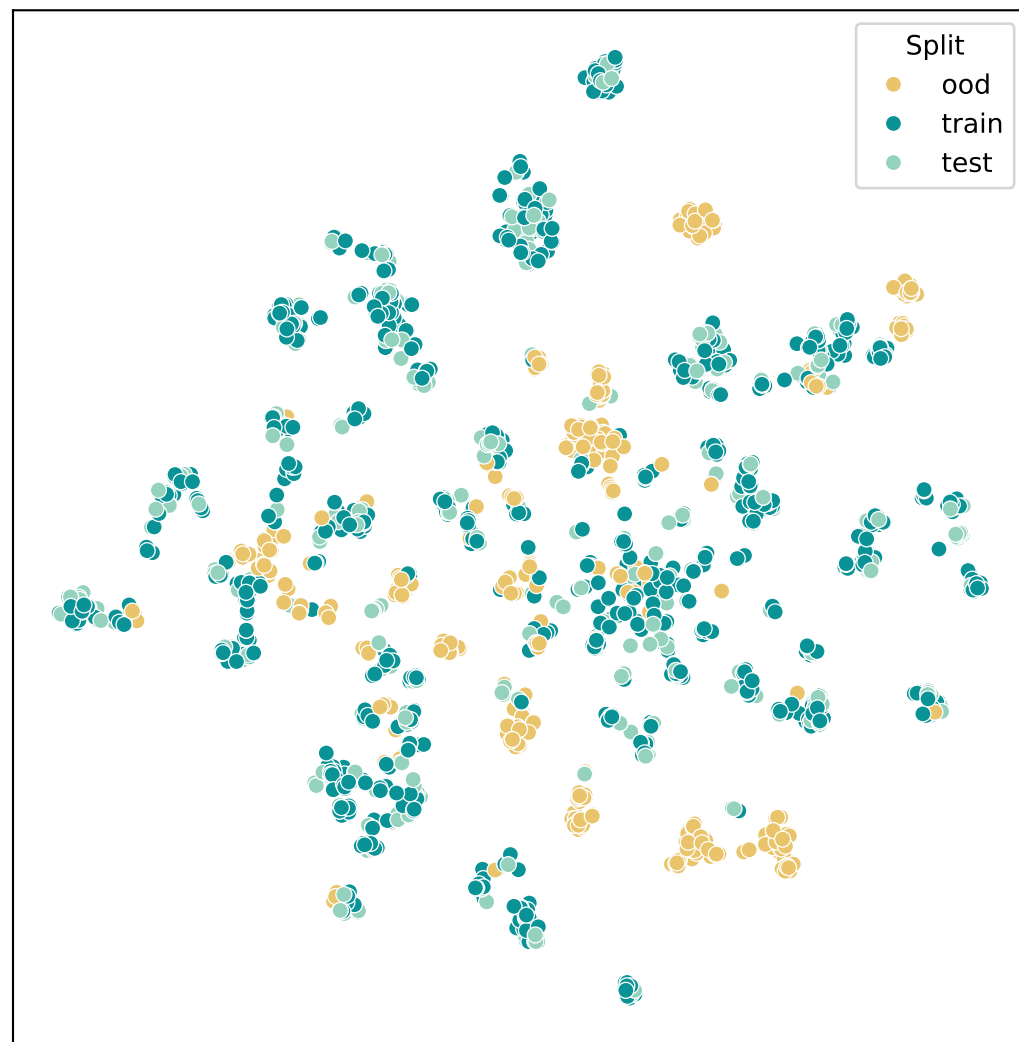
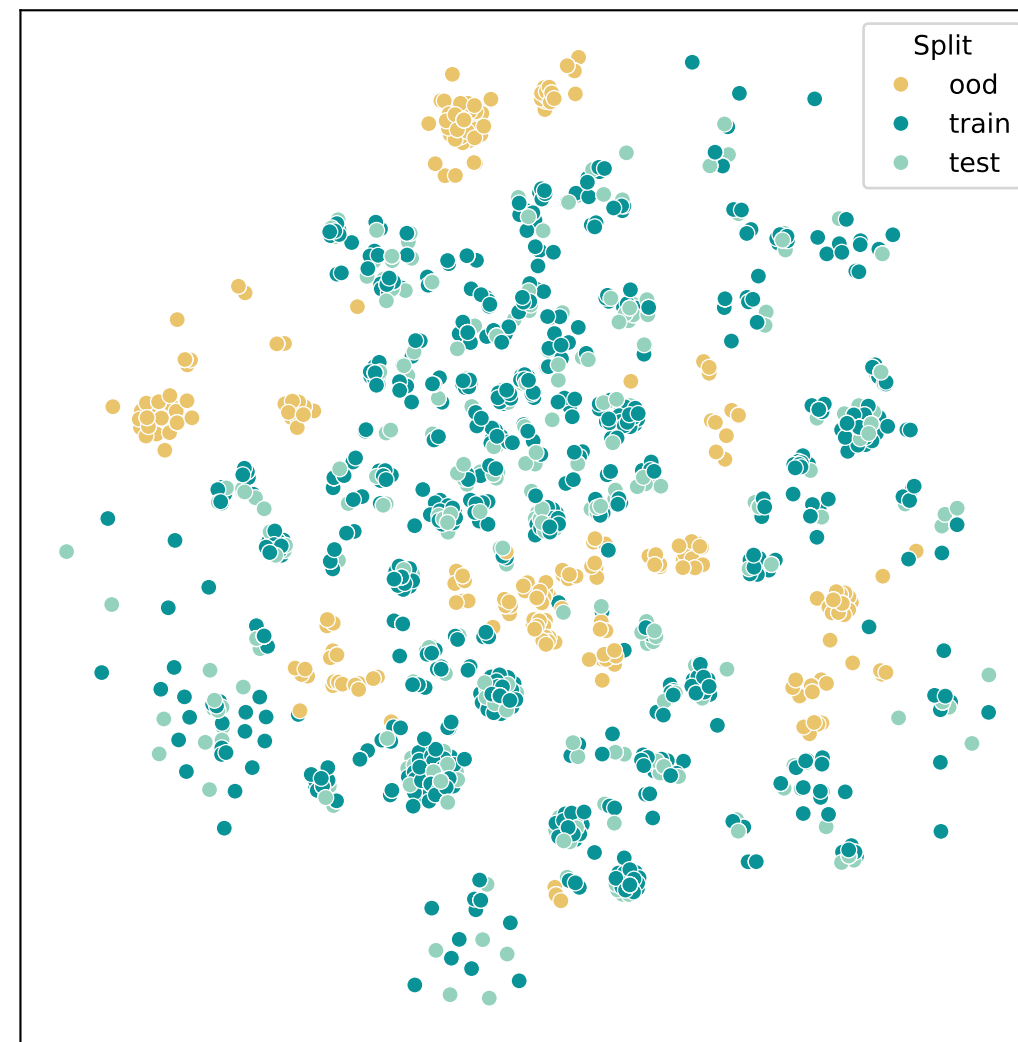


TSNE of CHEMBL237\_Ki (n=2460)



Whole molecule ECFPs



Cyclic skeleton ECFPs