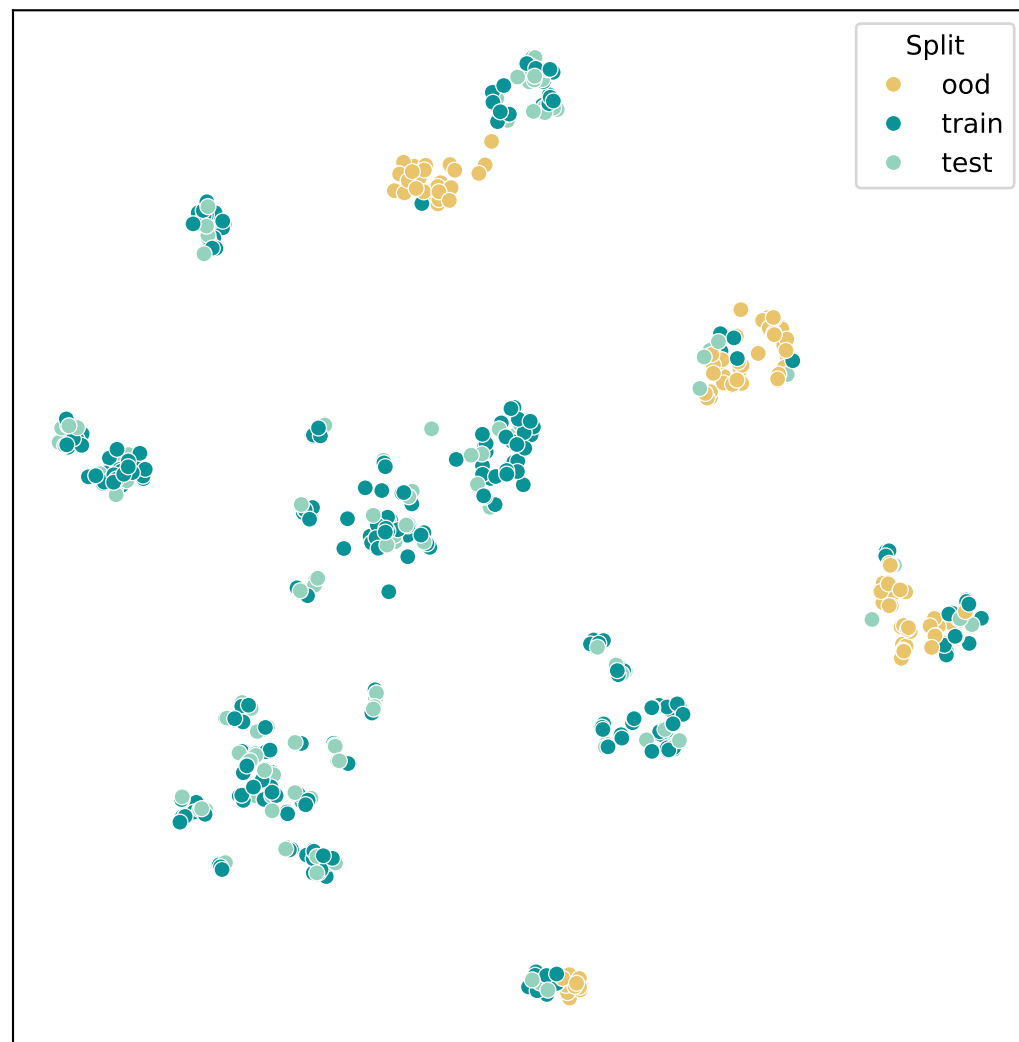
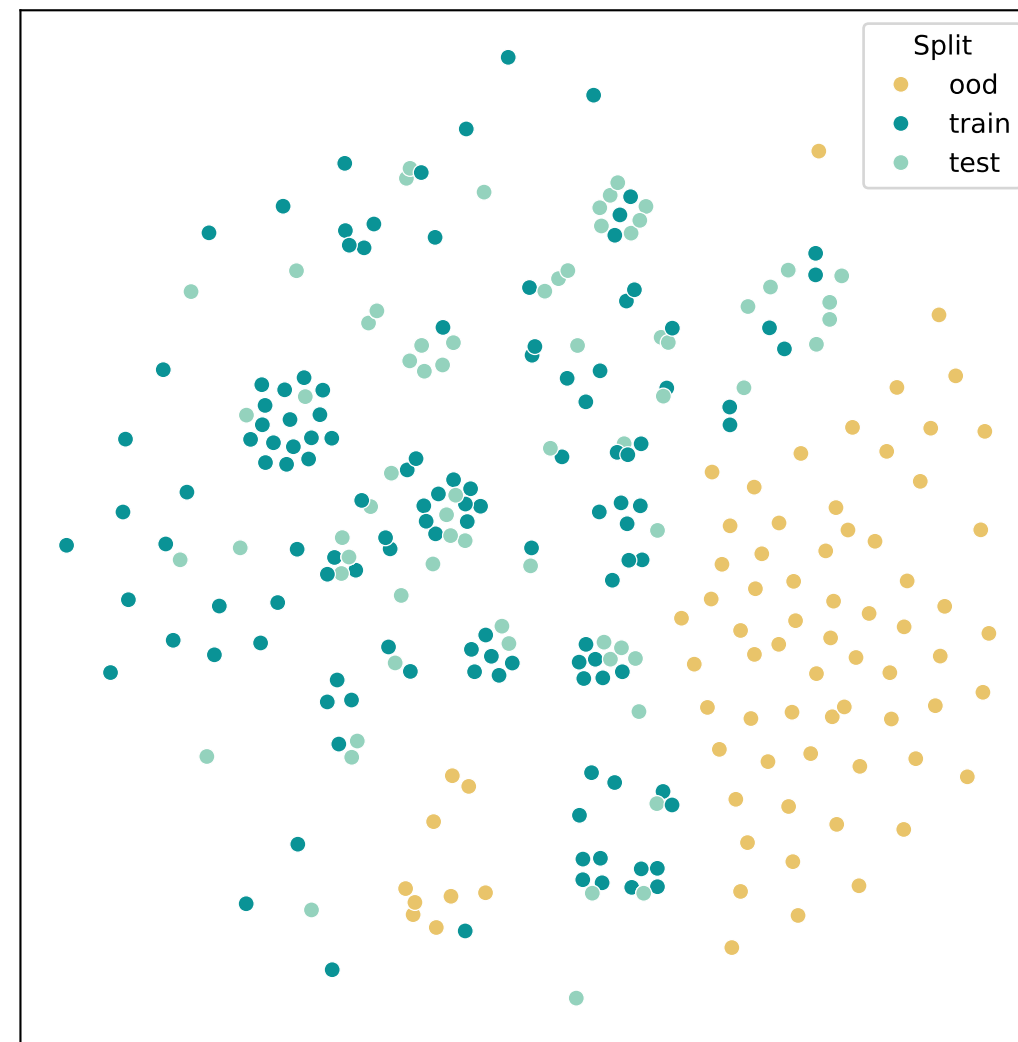


TSNE of CHEMBL2047\_EC50 (n=623)



Whole molecule ECFPs



Cyclic skeleton ECFPs