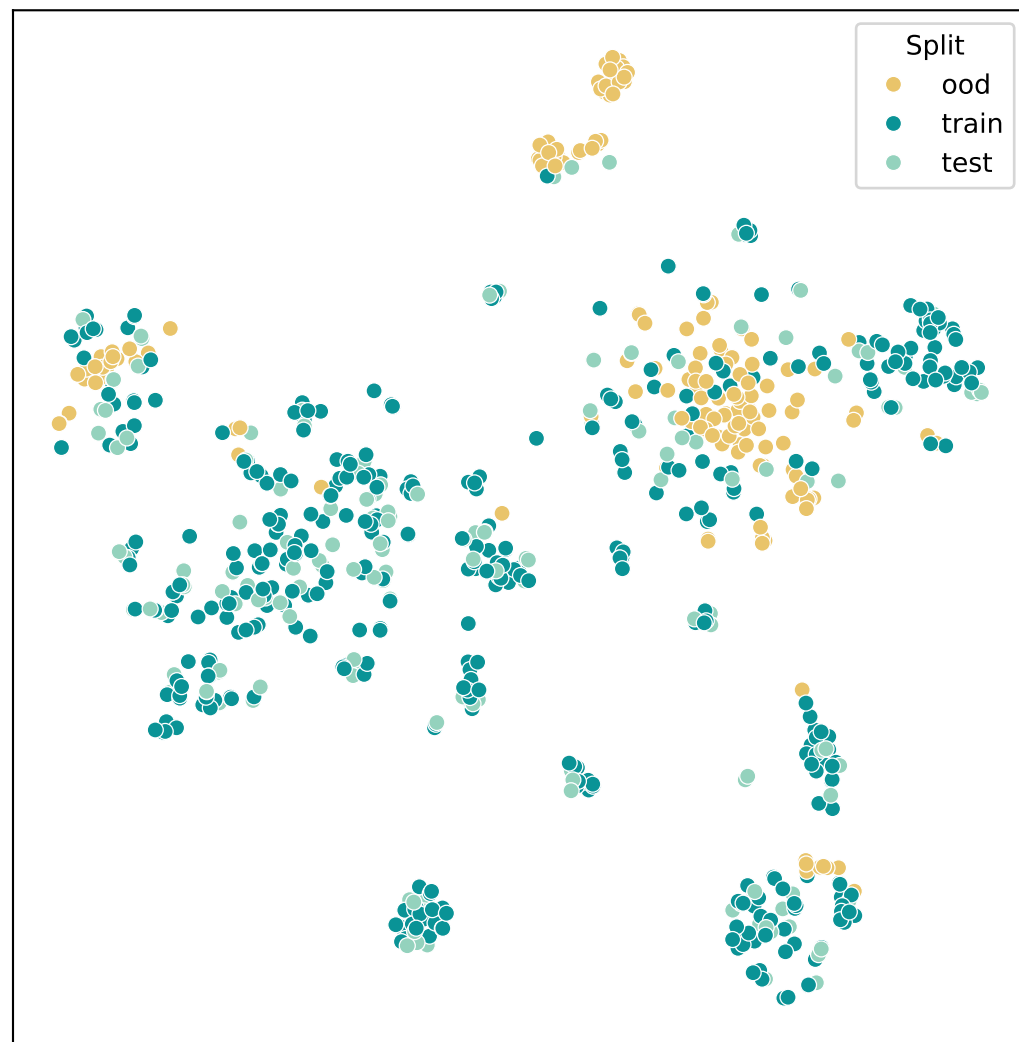
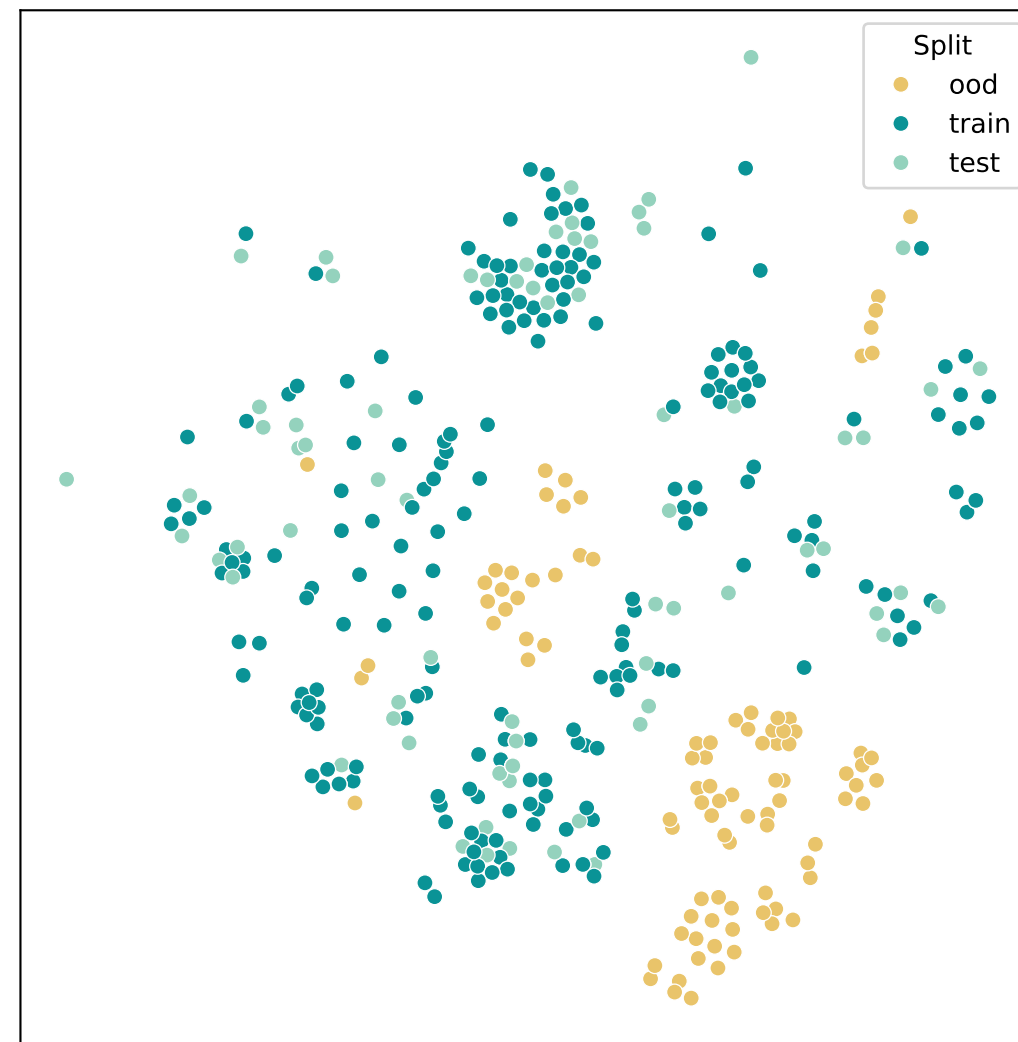


TSNE of CHEMBL1862_Ki (n=771)



Whole molecule ECFPs



Cyclic skeleton ECFPs