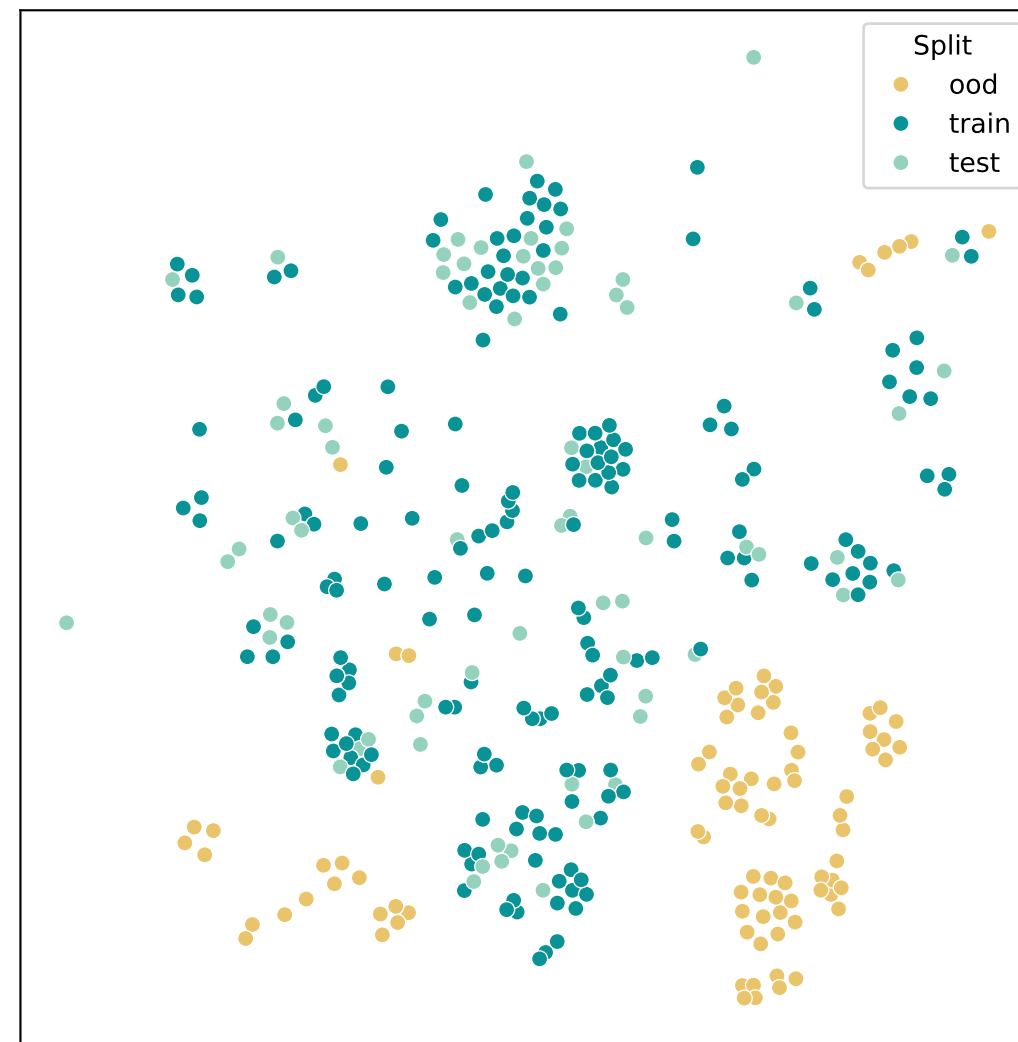


TSNE of CHEMBL1862\_Ki (n=771)



Whole molecule ECFPs



Cyclic skeleton ECFPs