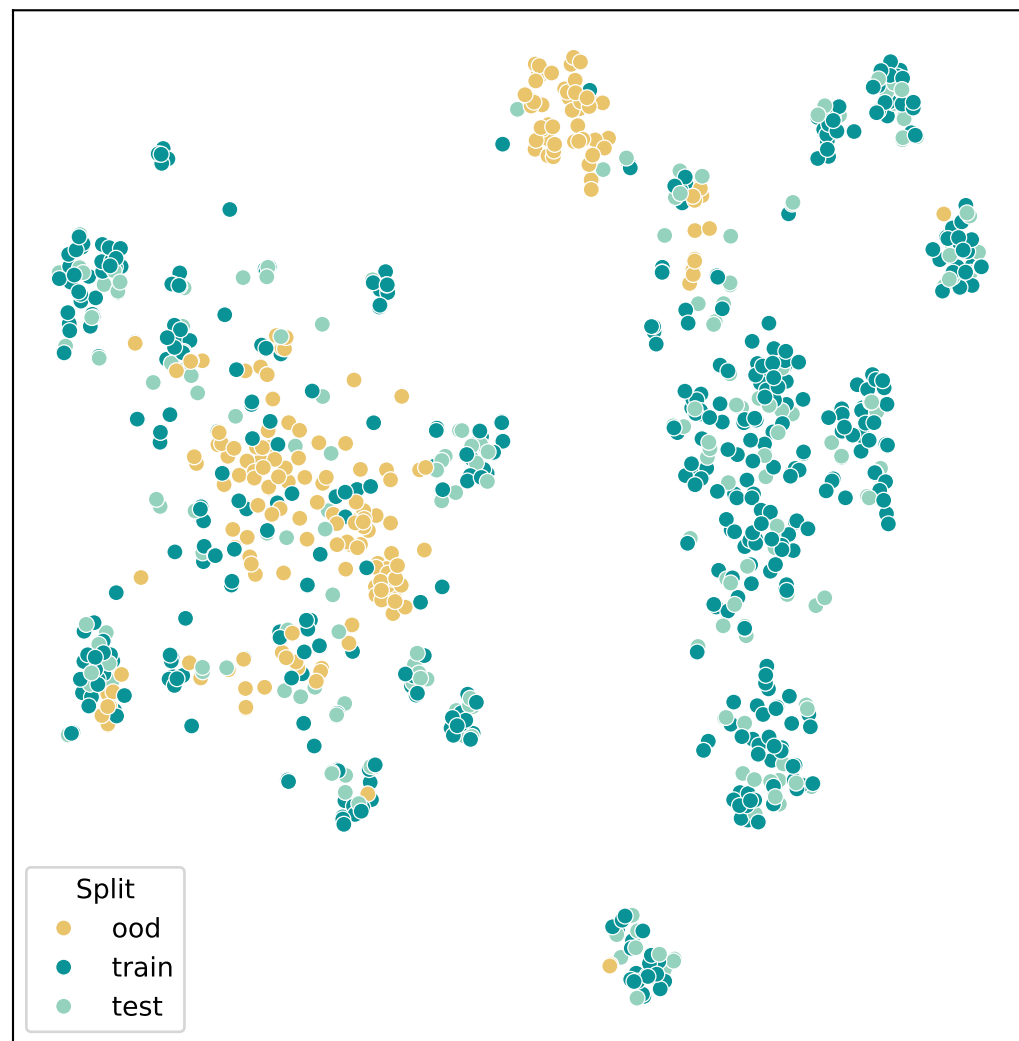


TSNE of CHEMBL2971_Ki (n=966)



Whole molecule ECFPs



Cyclic skeleton ECFPs