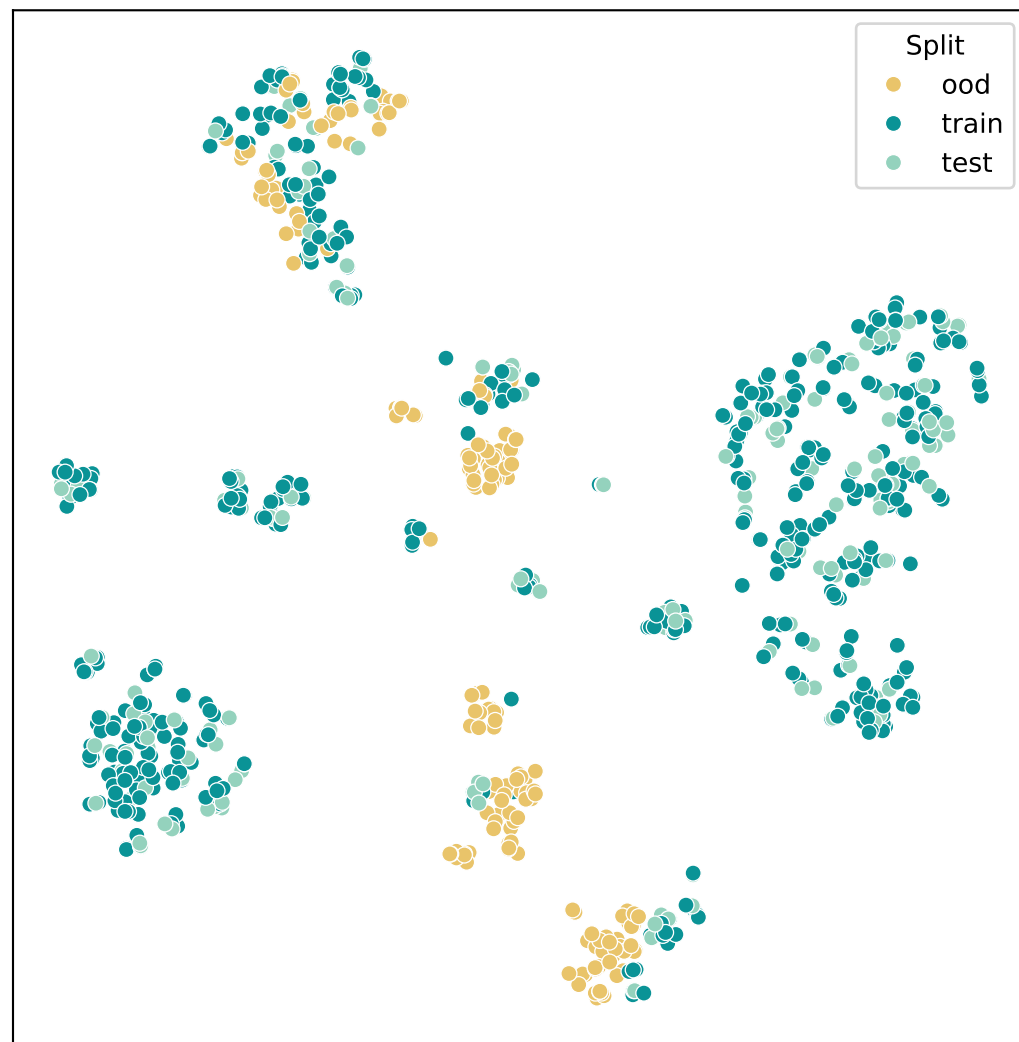
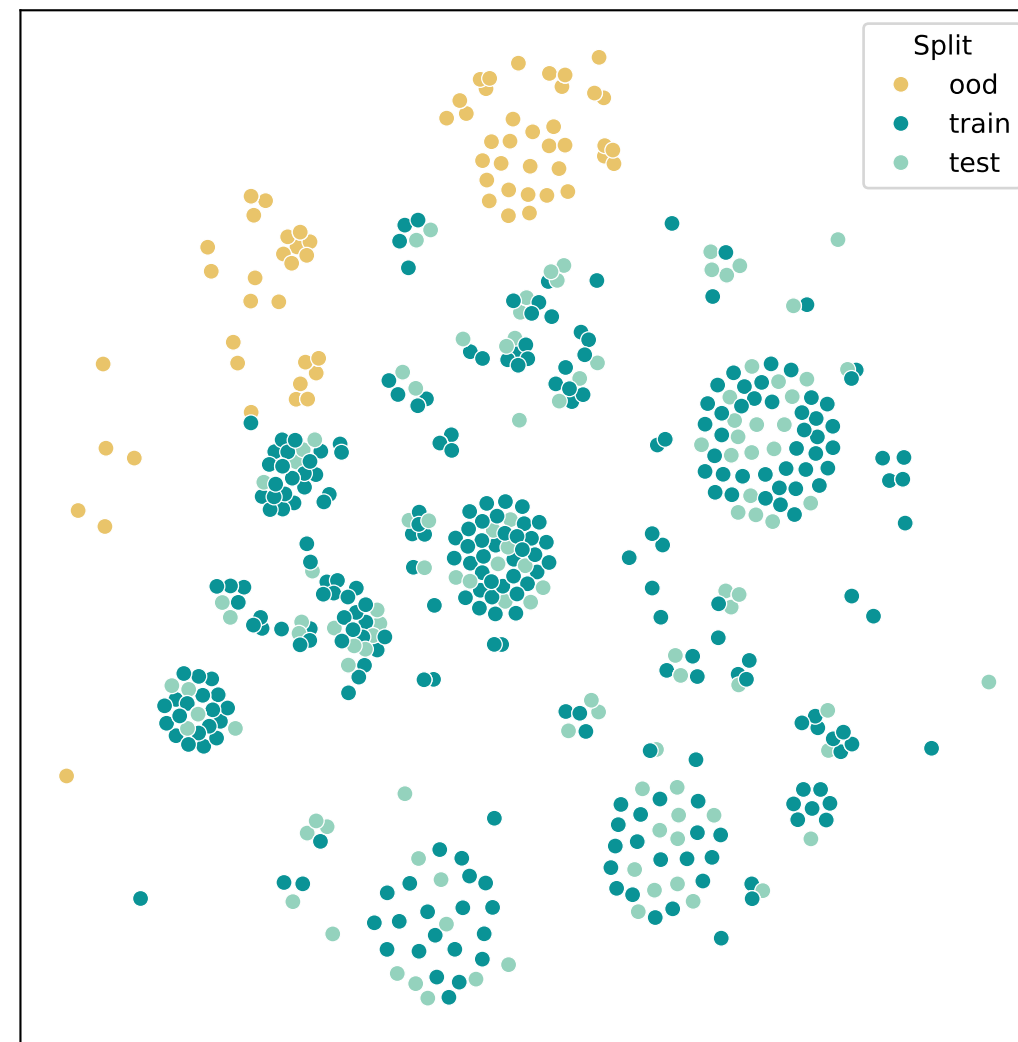


TSNE of CHEMBL4005_Ki (n=958)



Whole molecule ECFPs



Cyclic skeleton ECFPs