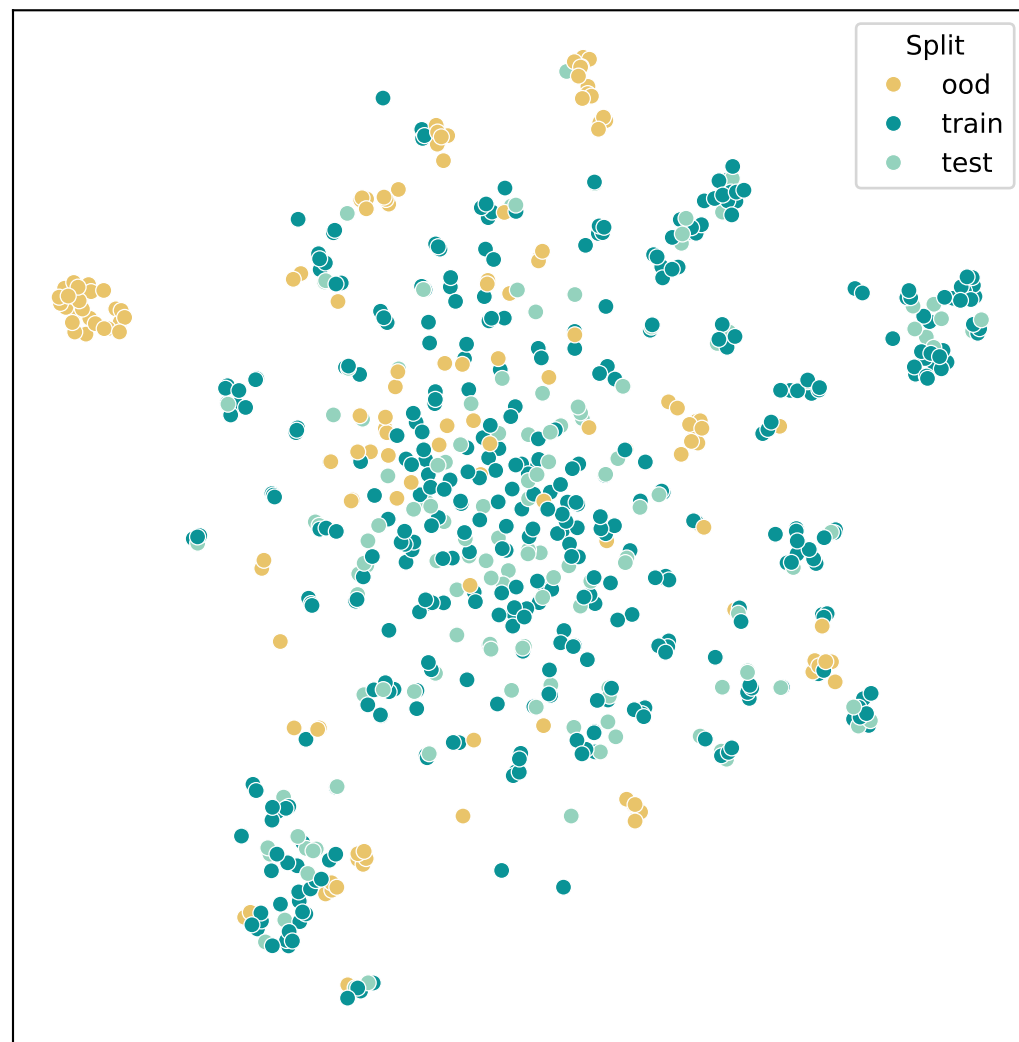
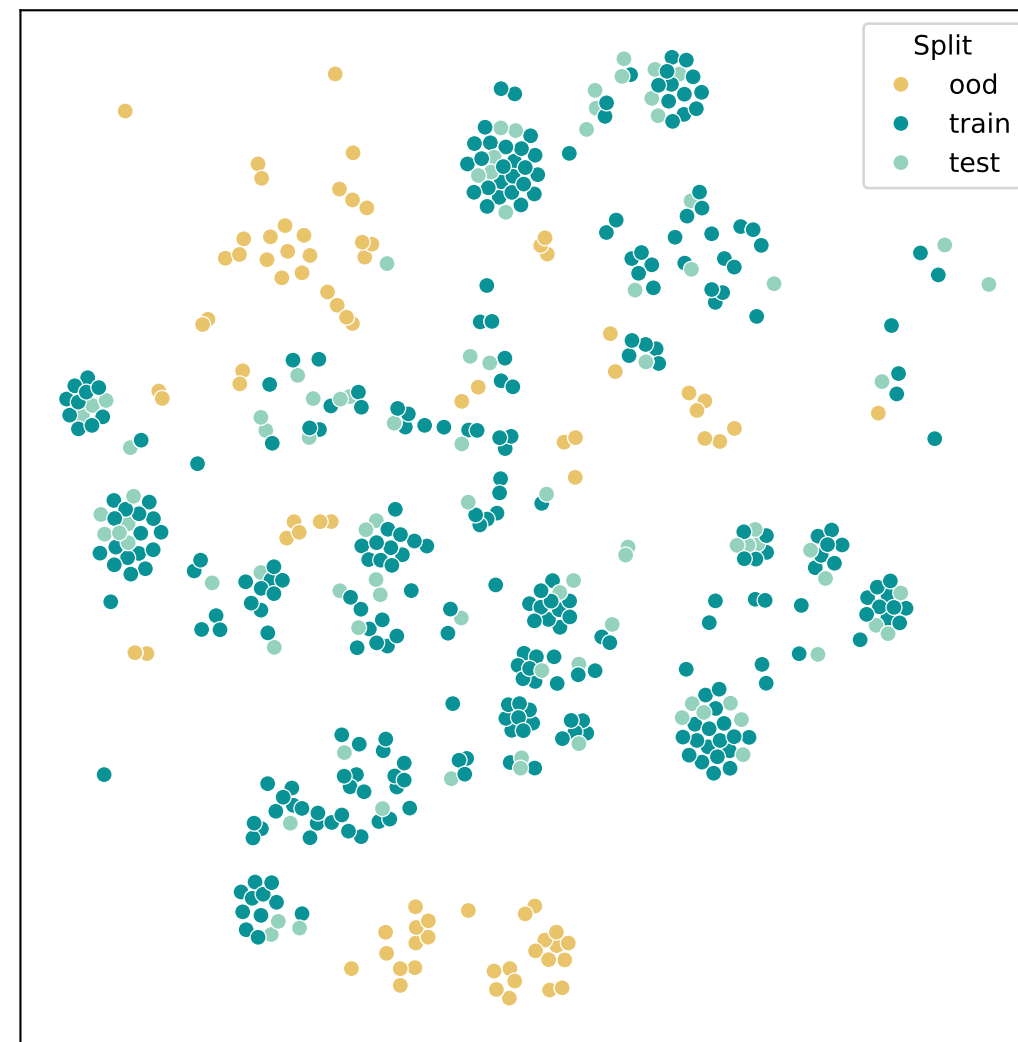


TSNE of CHEMBL4203_Ki (n=717)



Whole molecule ECFPs



Cyclic skeleton ECFPs