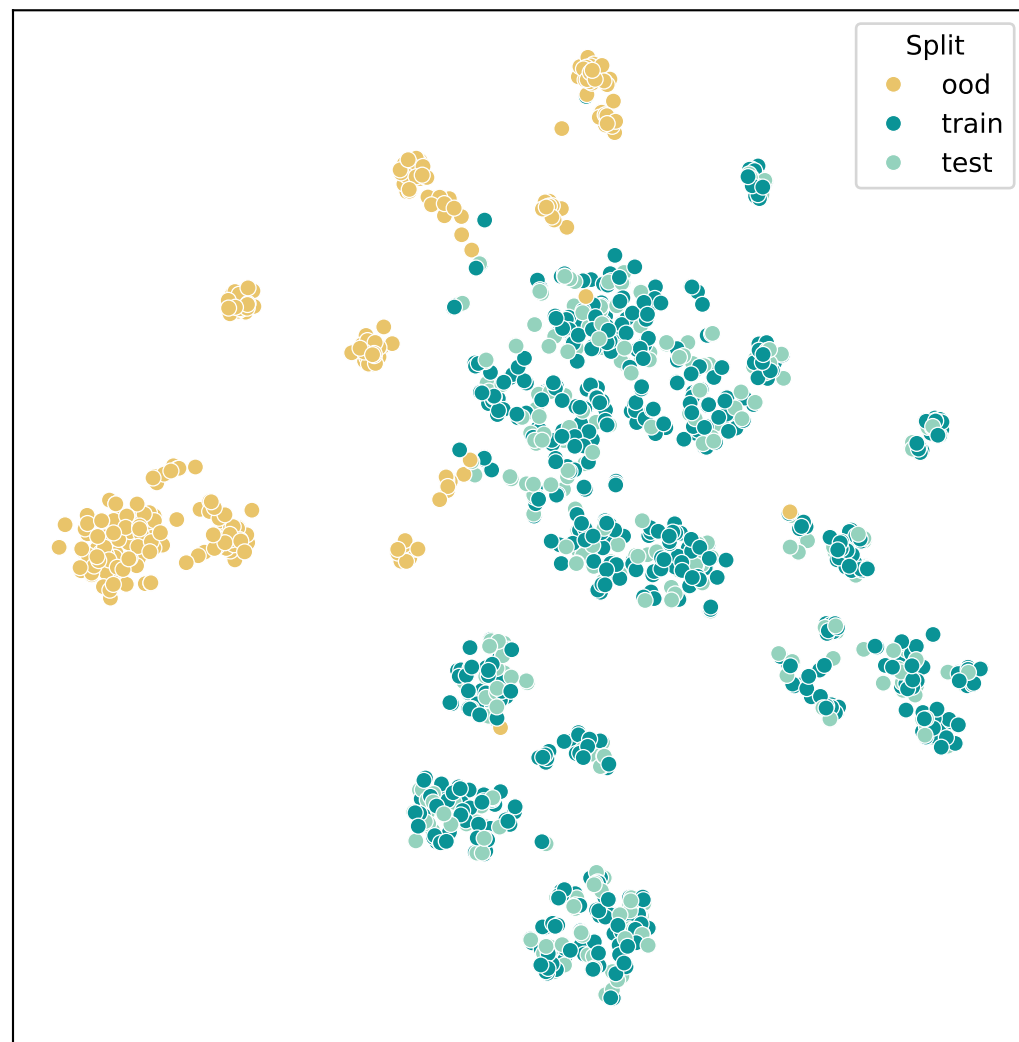
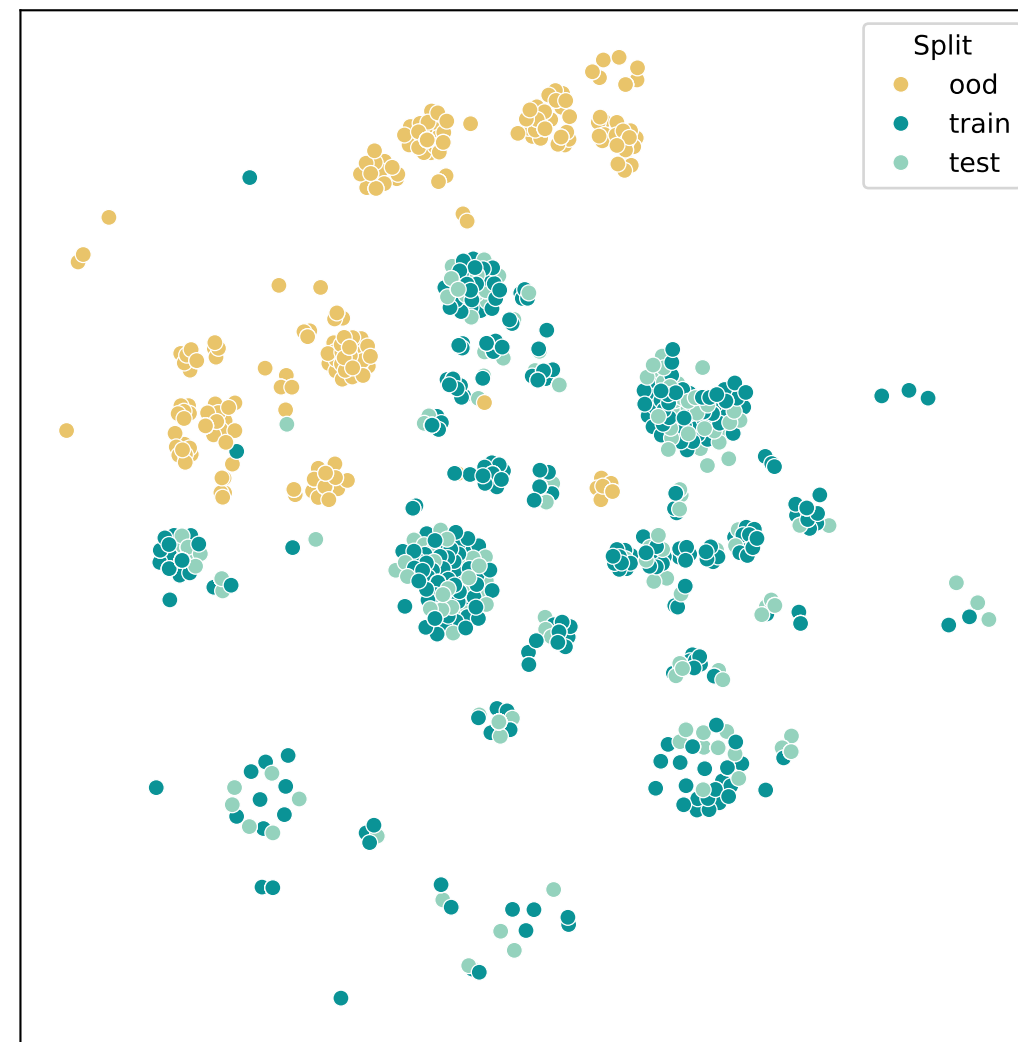


TSNE of CHEMBL4792_Ki (n=1467)



Whole molecule ECFPs



Cyclic skeleton ECFPs