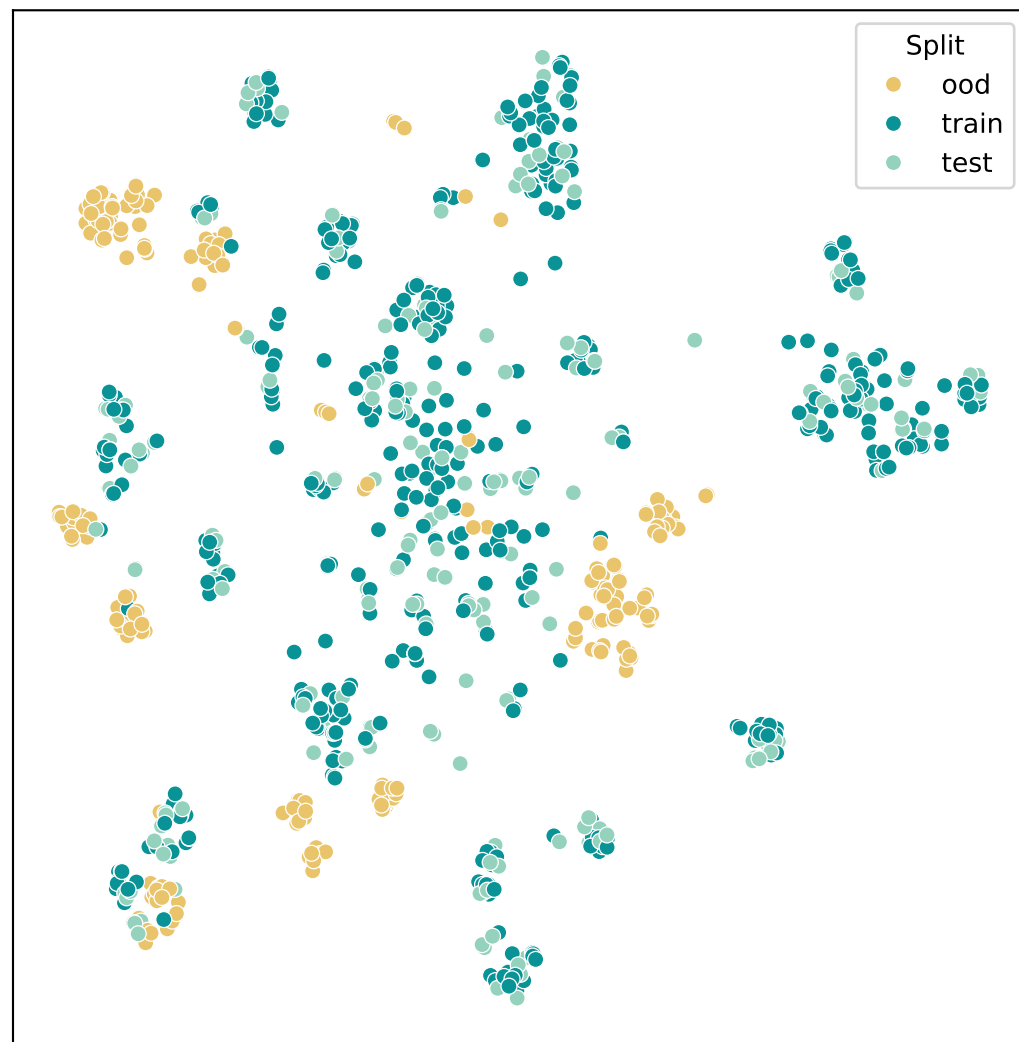
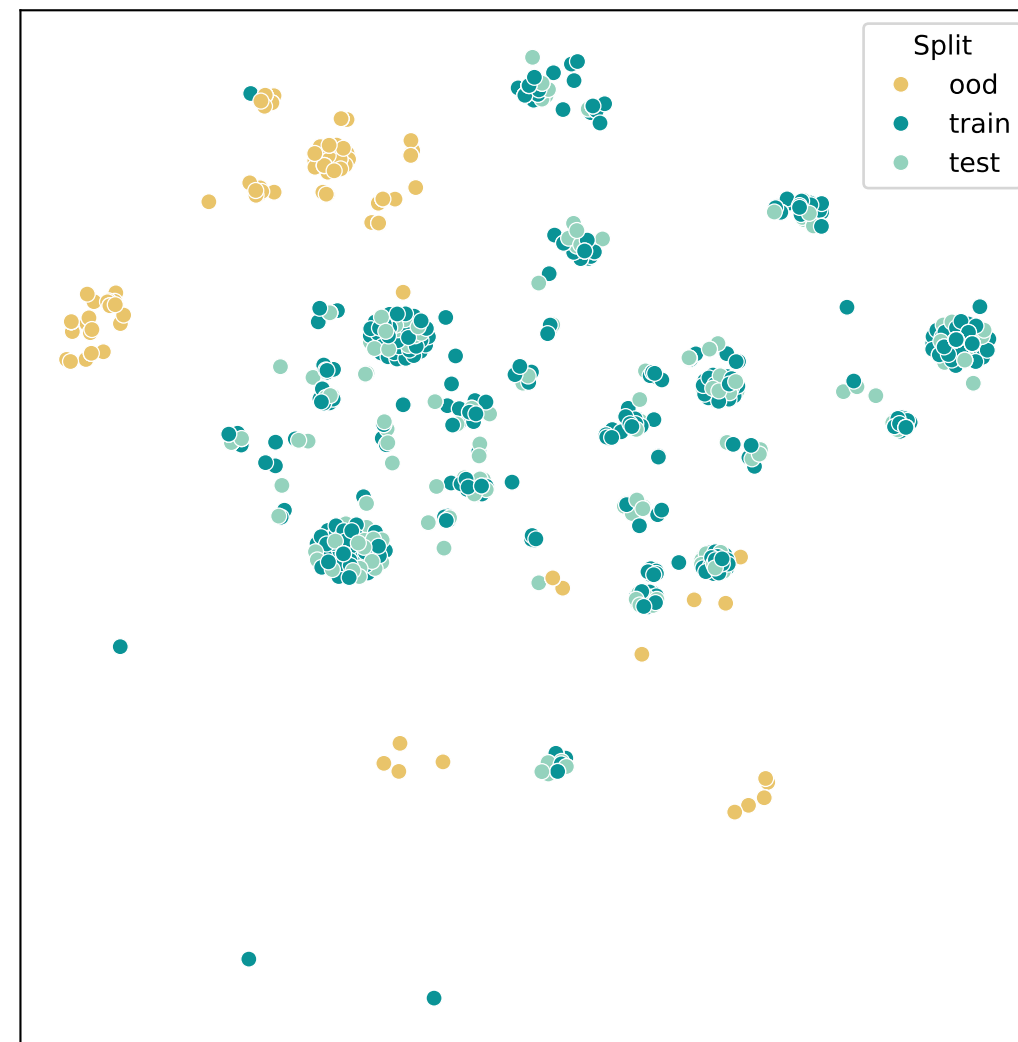


TSNE of CHEMBL238_Ki (n=1015)



Whole molecule ECFPs



Cyclic skeleton ECFPs