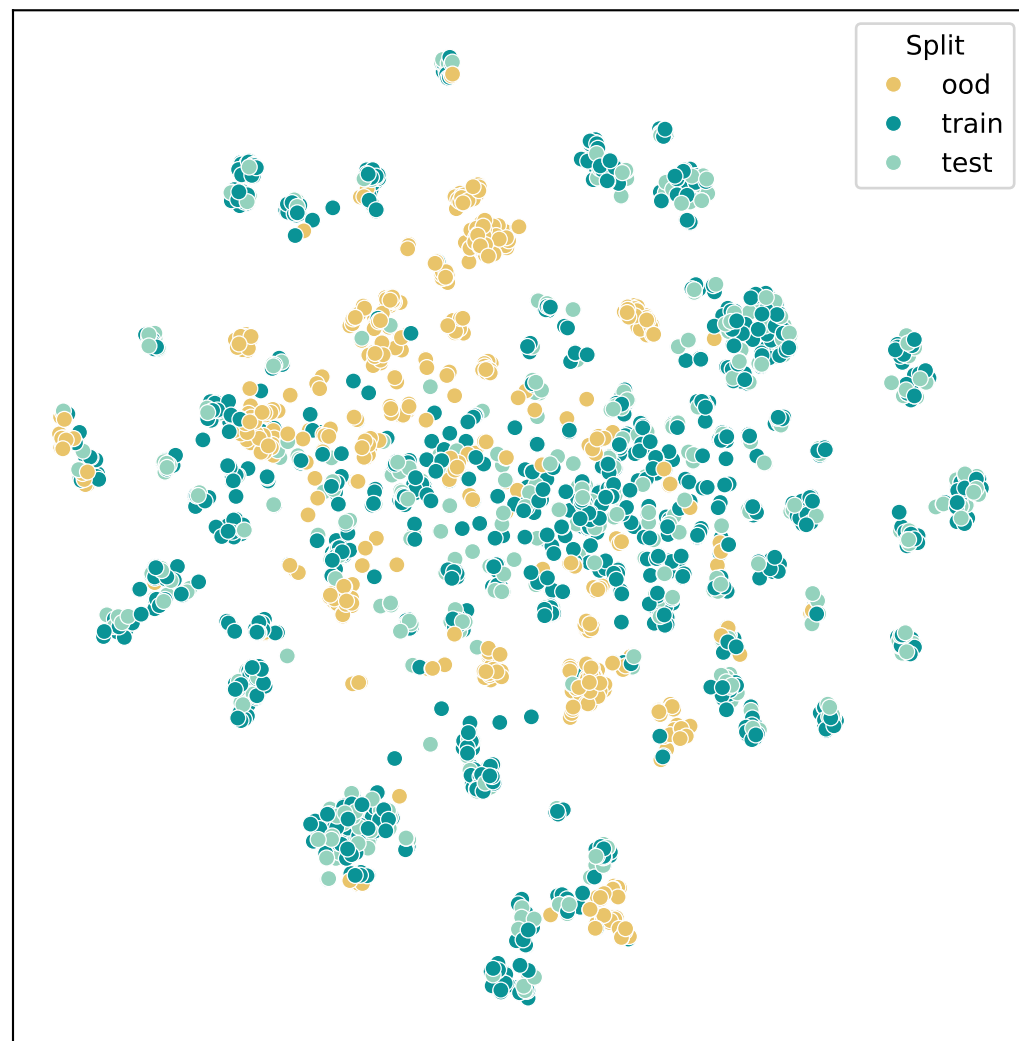
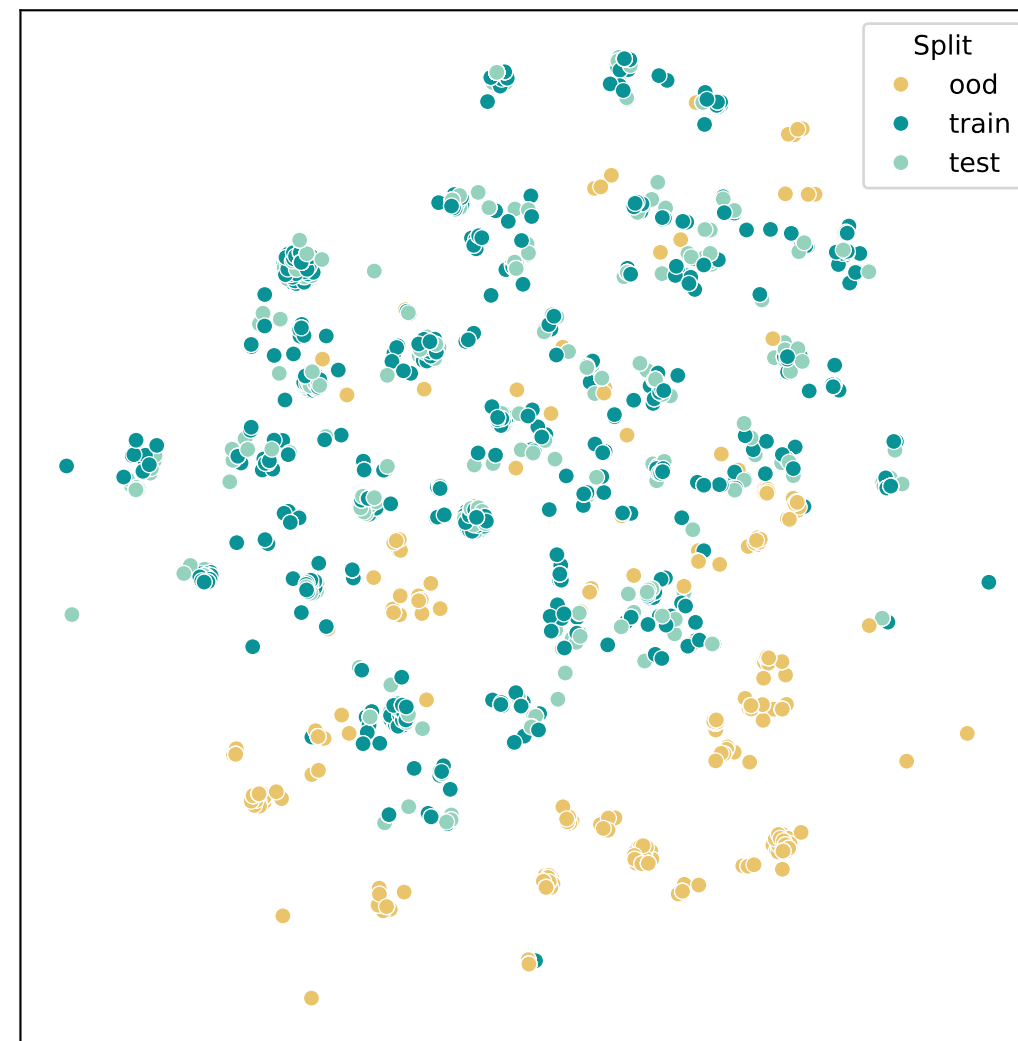


TSNE of CHEMBL214_Ki (n=3236)



Whole molecule ECFPs



Cyclic skeleton ECFPs