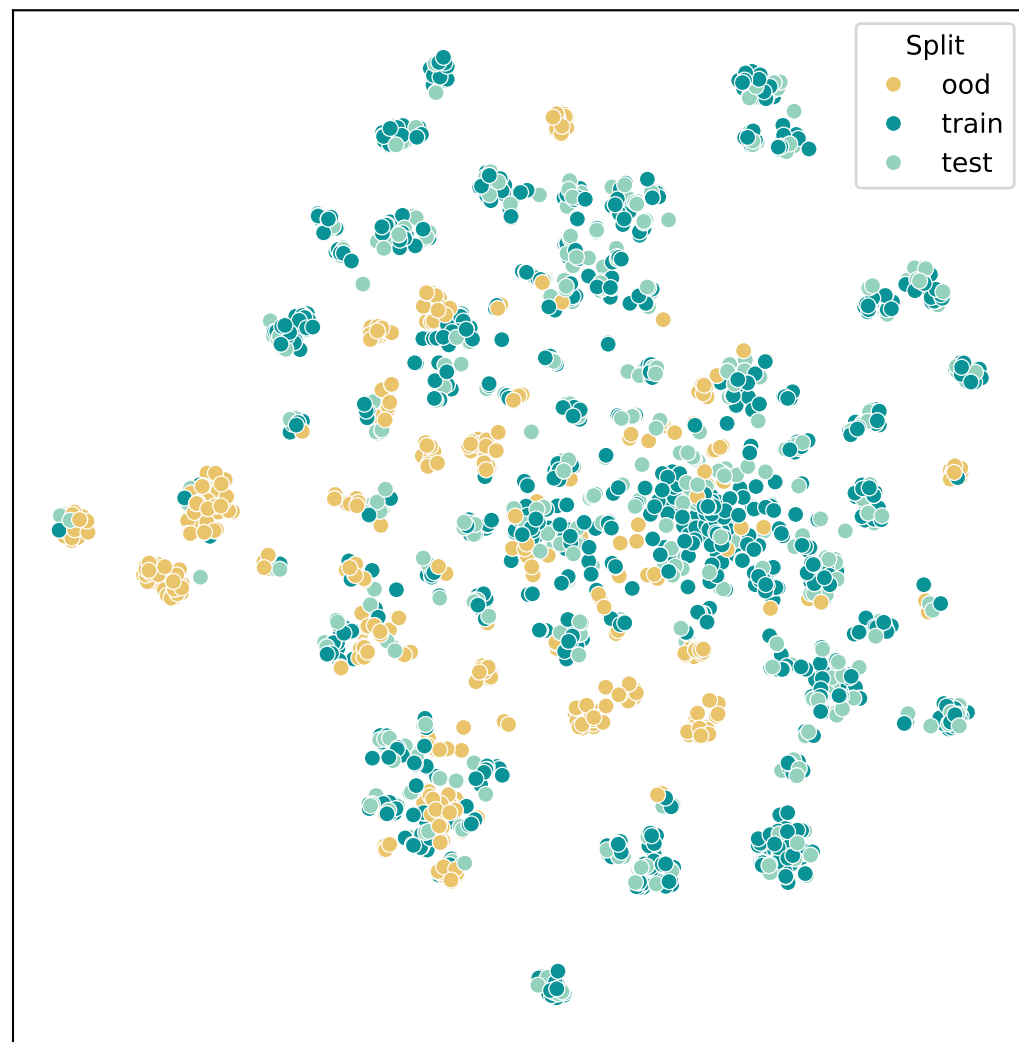
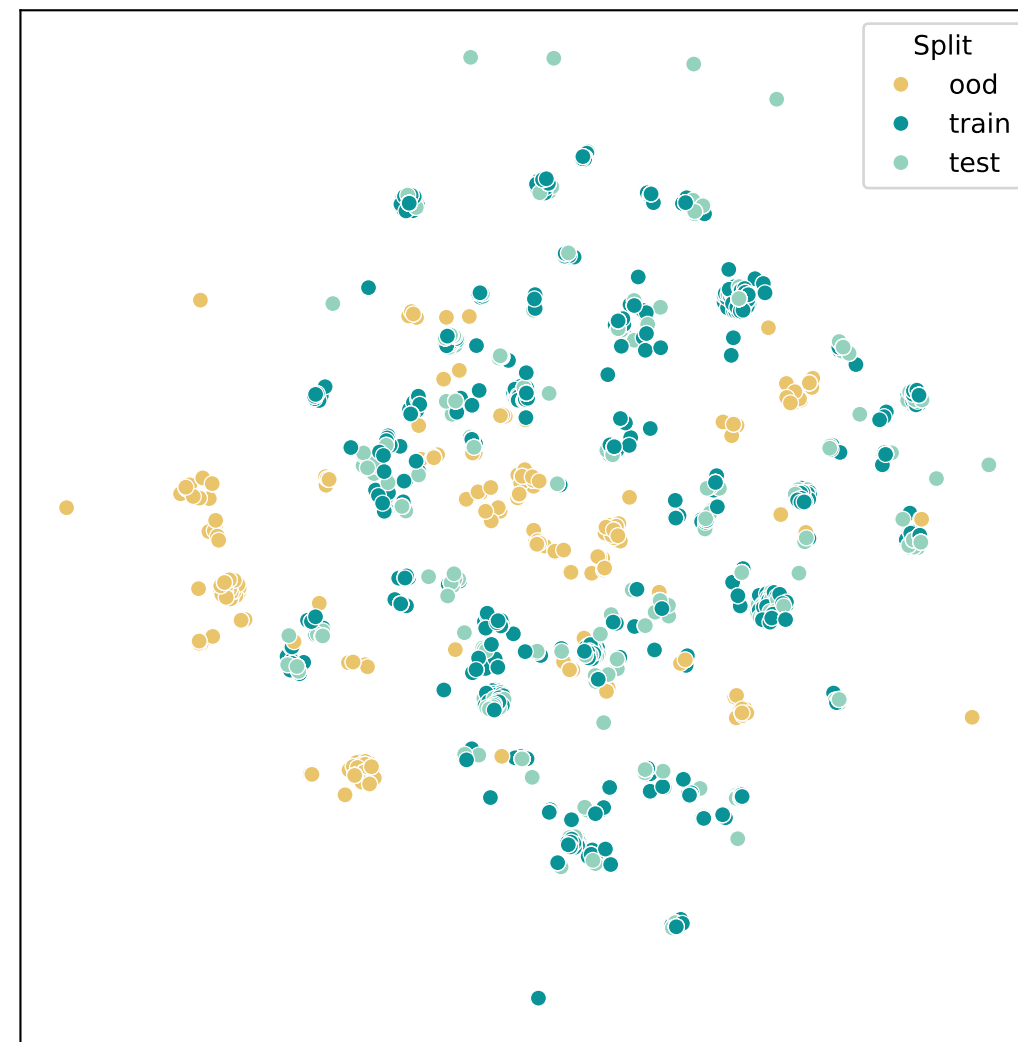


TSNE of CHEMBL264_Ki (n=2835)



Whole molecule ECFPs



Cyclic skeleton ECFPs