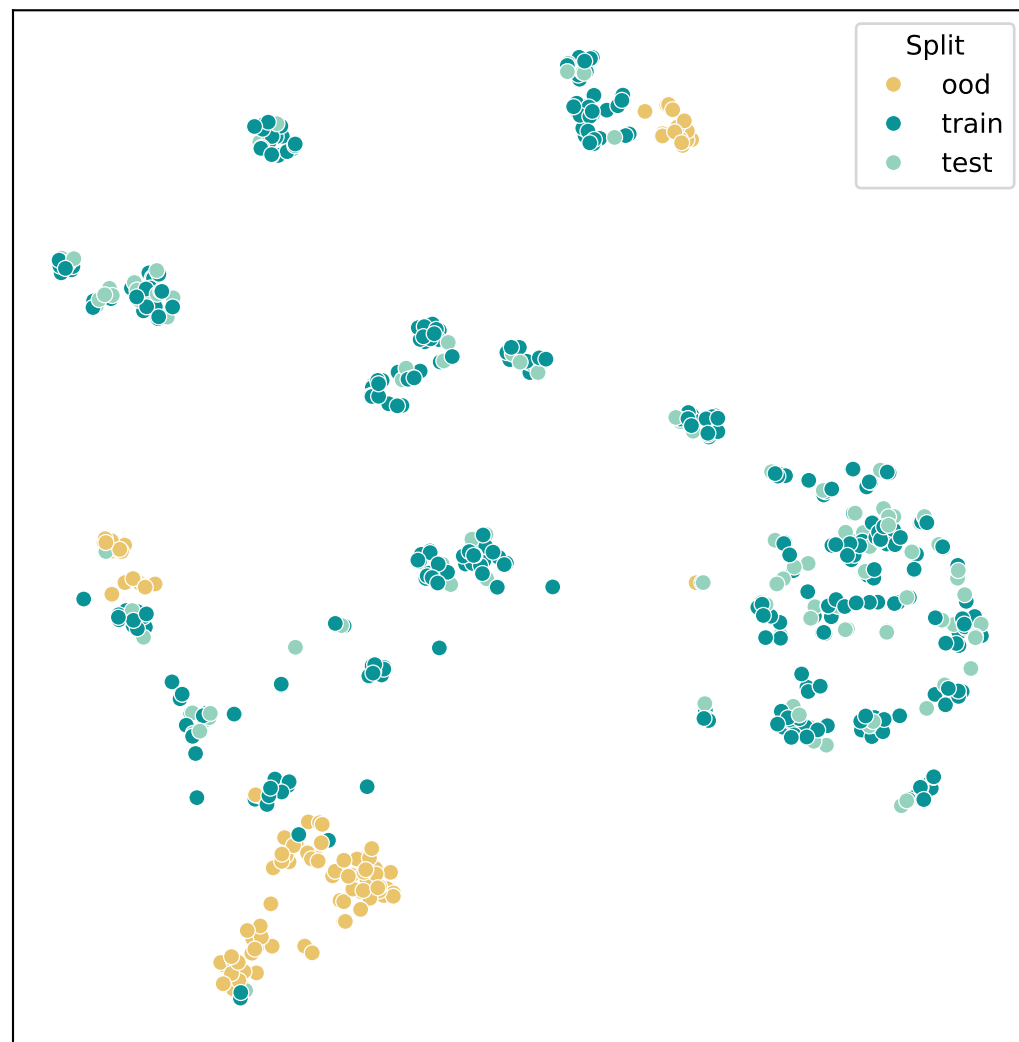
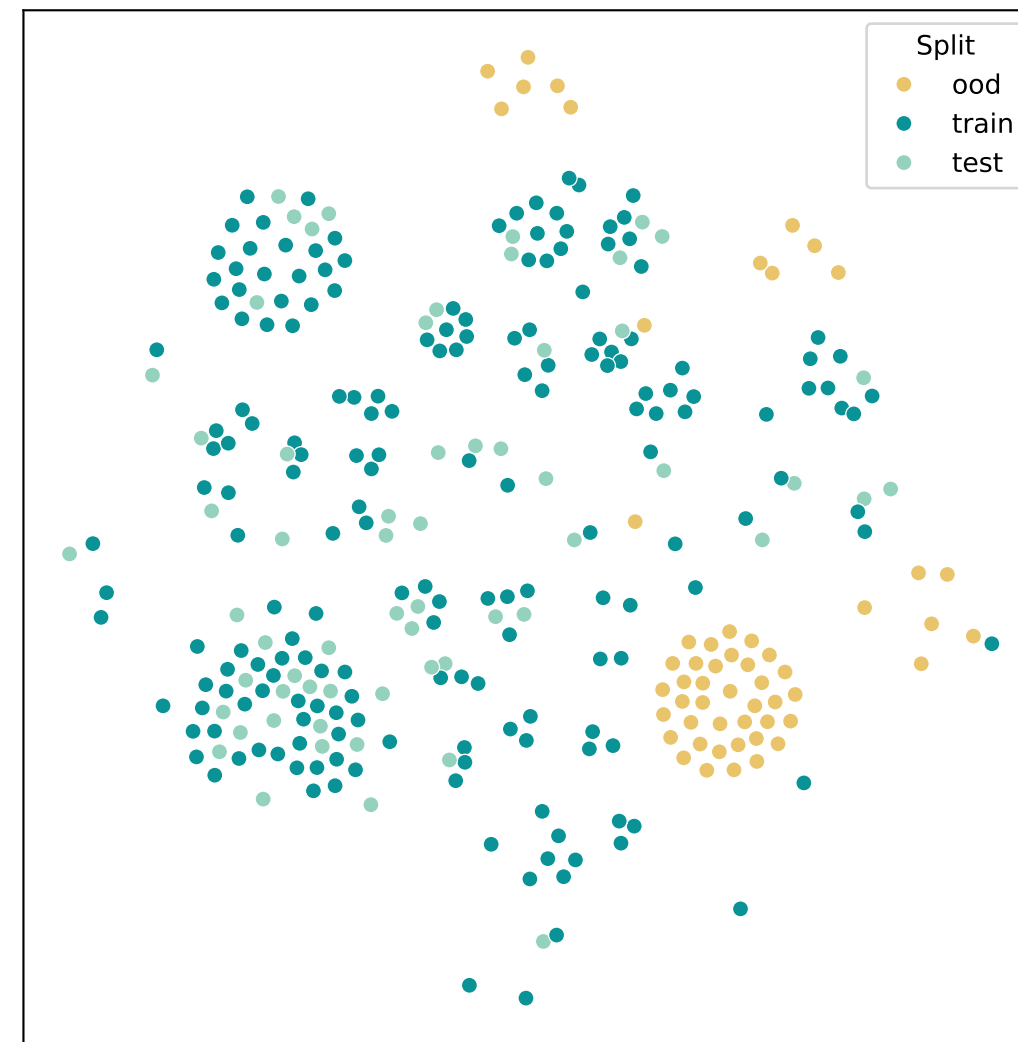


TSNE of CHEMBL4616_EC50 (n=638)



Whole molecule ECFPs



Cyclic skeleton ECFPs