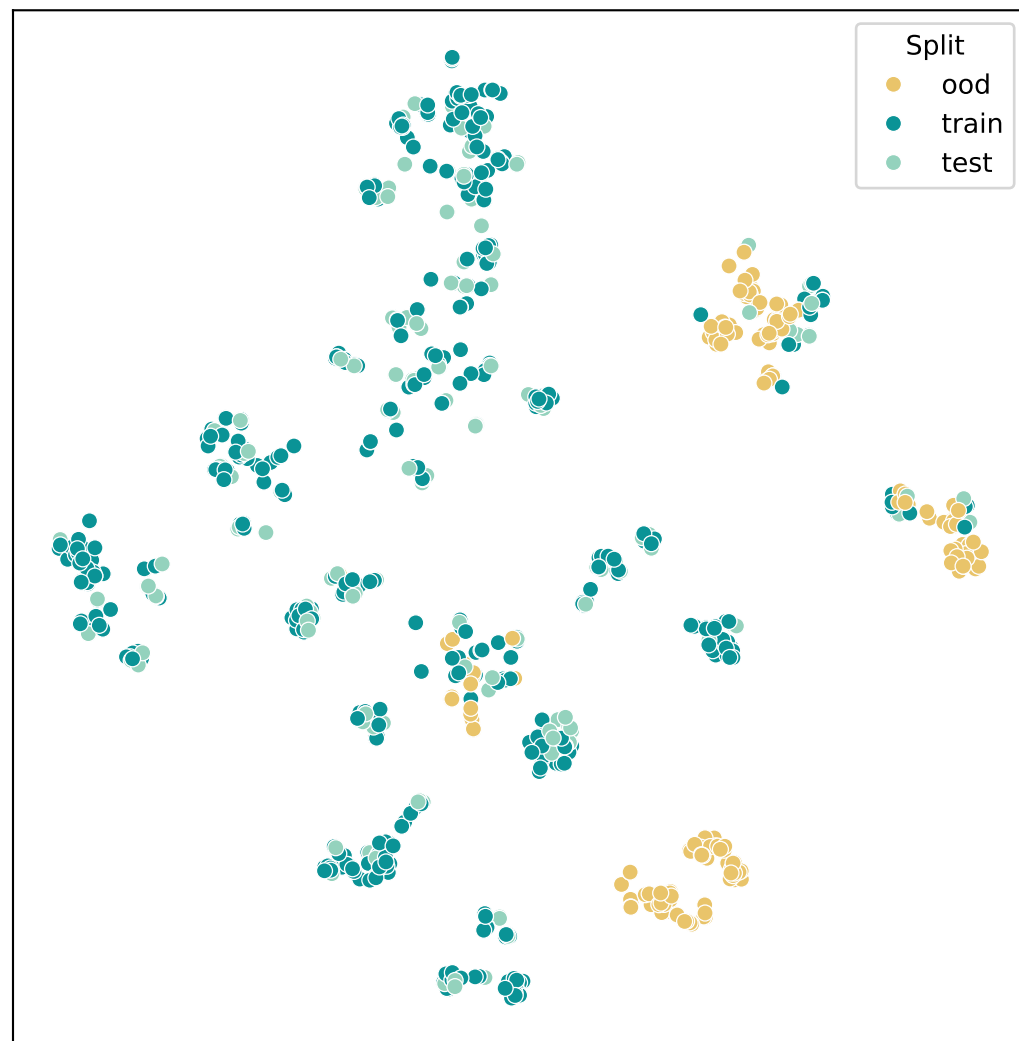
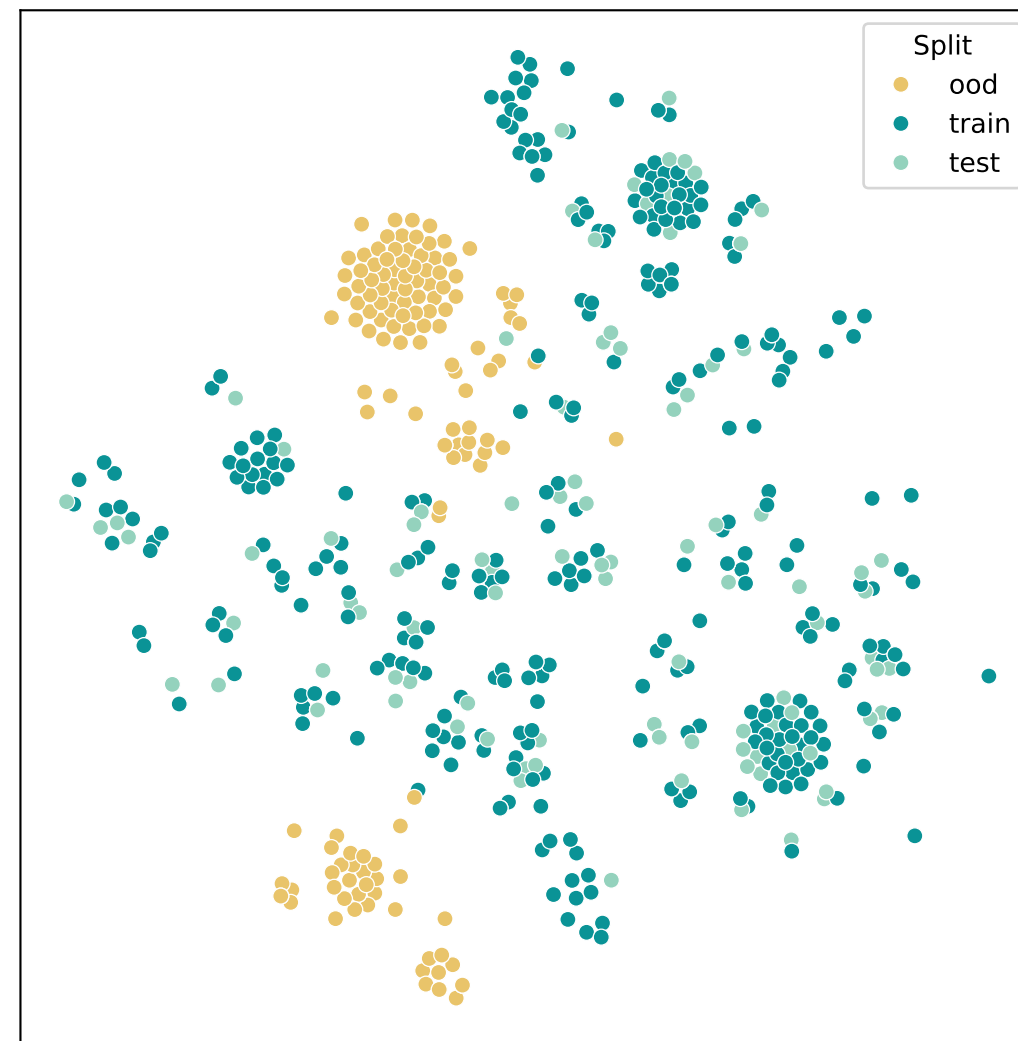


TSNE of CHEMBL237_EC50 (n=914)



Whole molecule ECFPs



Cyclic skeleton ECFPs