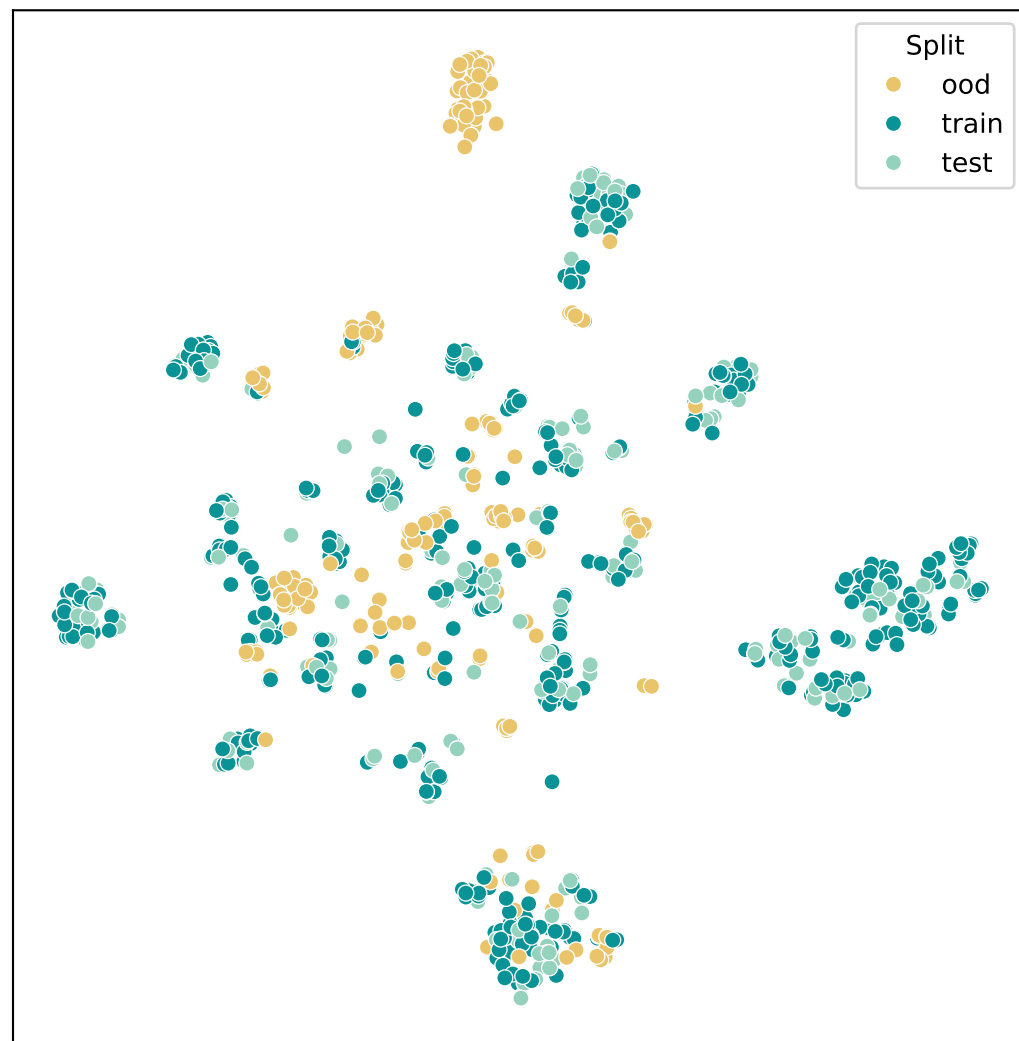
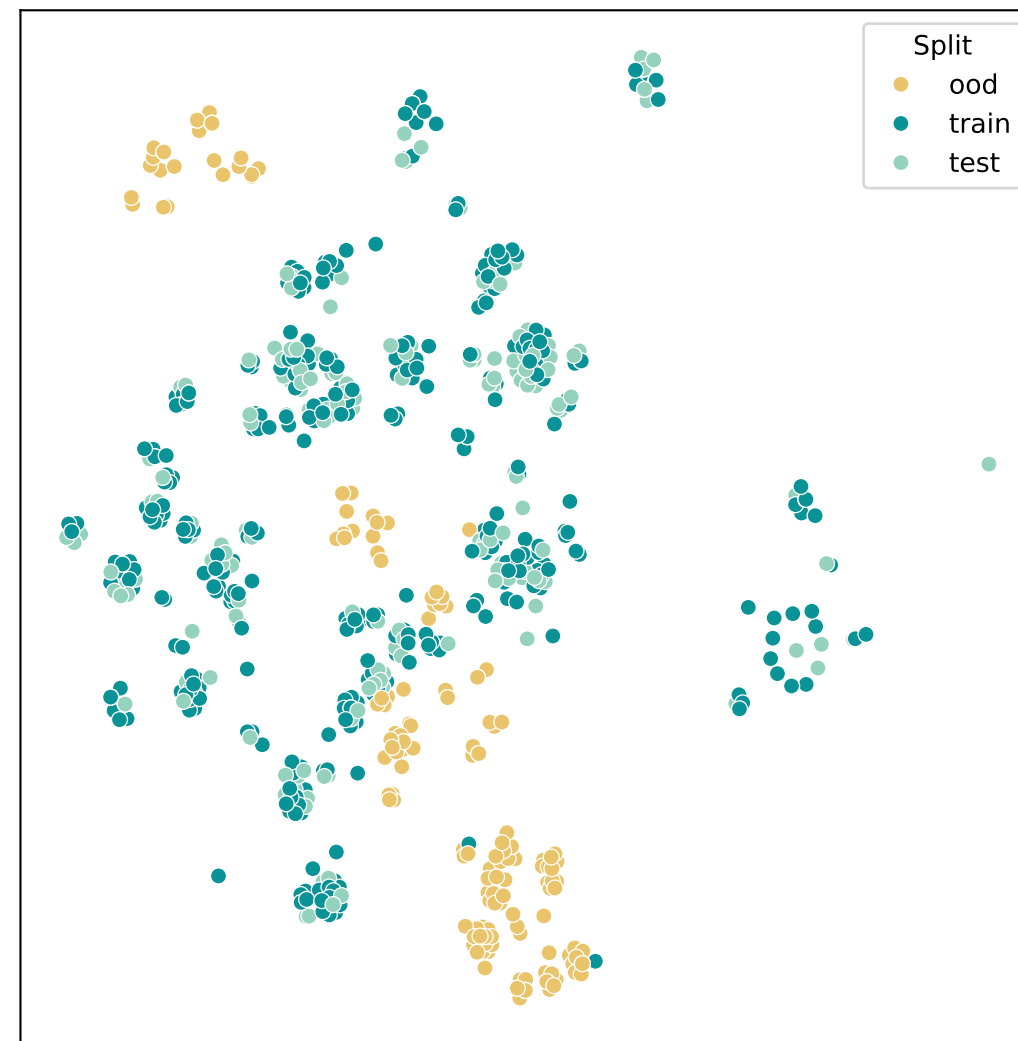


TSNE of CHEMBL218_EC50 (n=1002)



Whole molecule ECFPs



Cyclic skeleton ECFPs