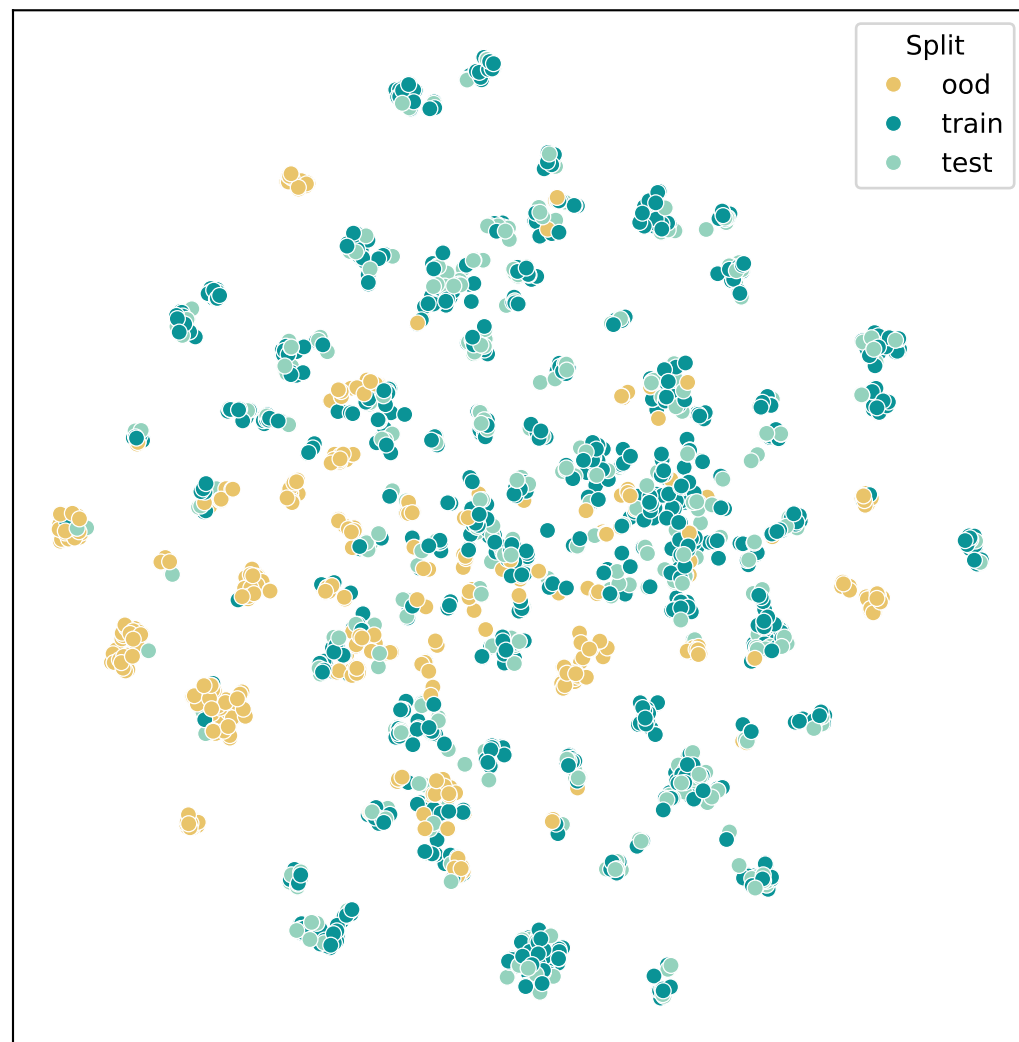
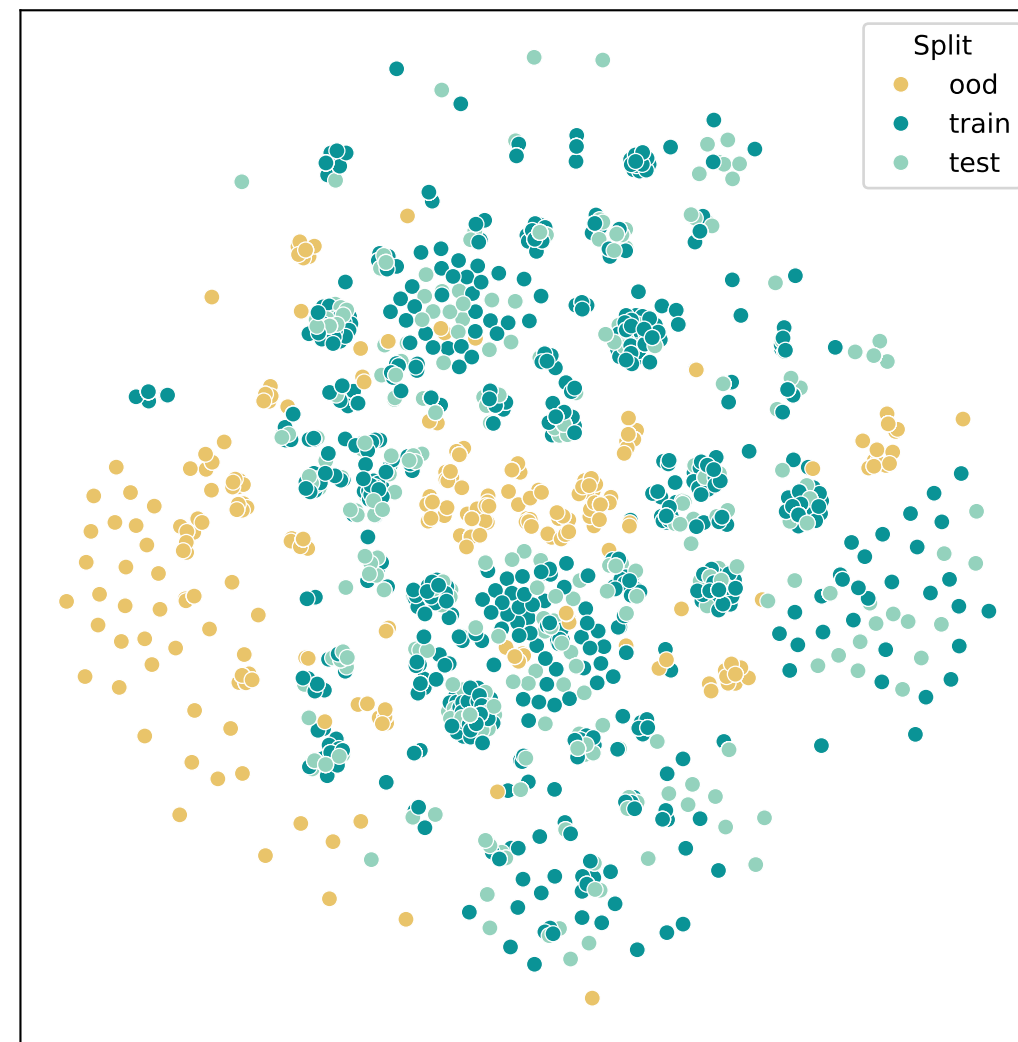


TSNE of CHEMBL264\_Ki (n=2835)



Whole molecule ECFPs



Cyclic skeleton ECFPs