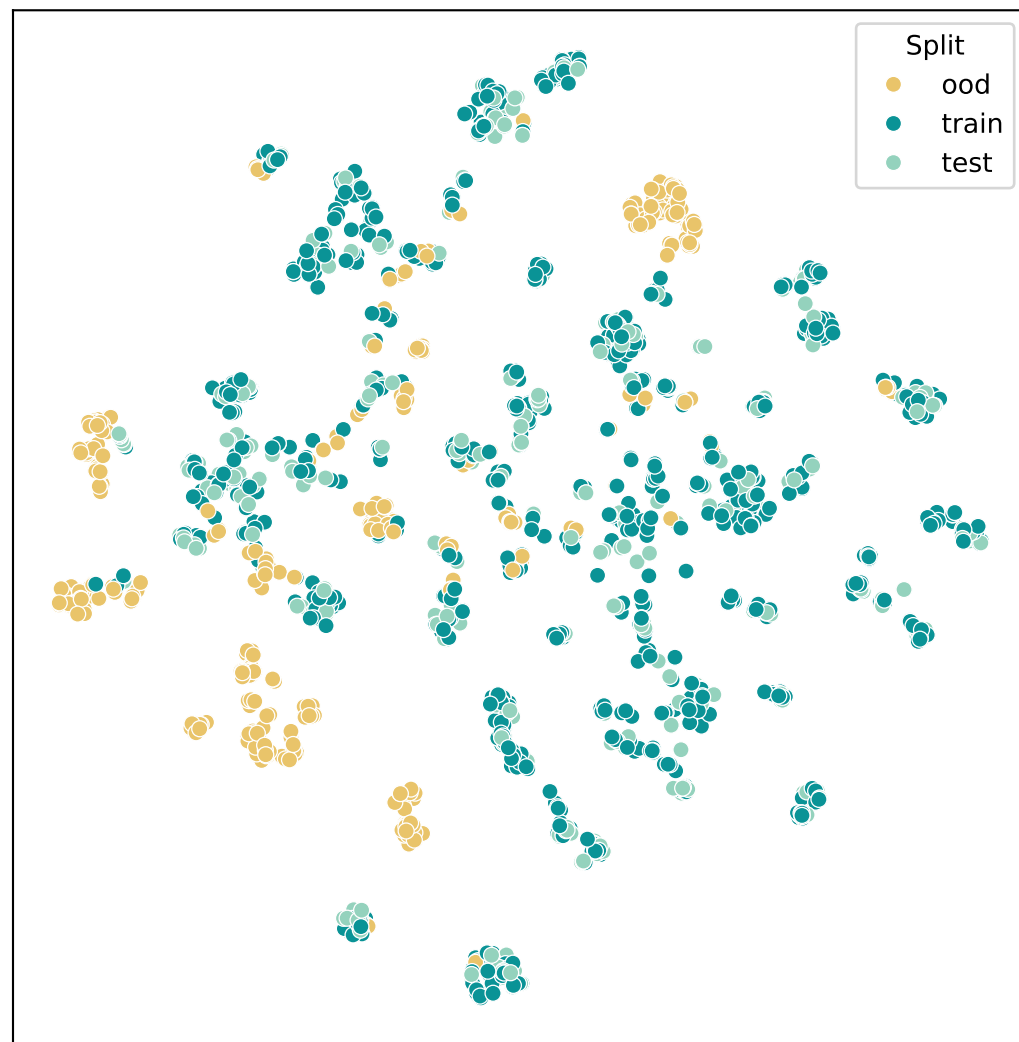
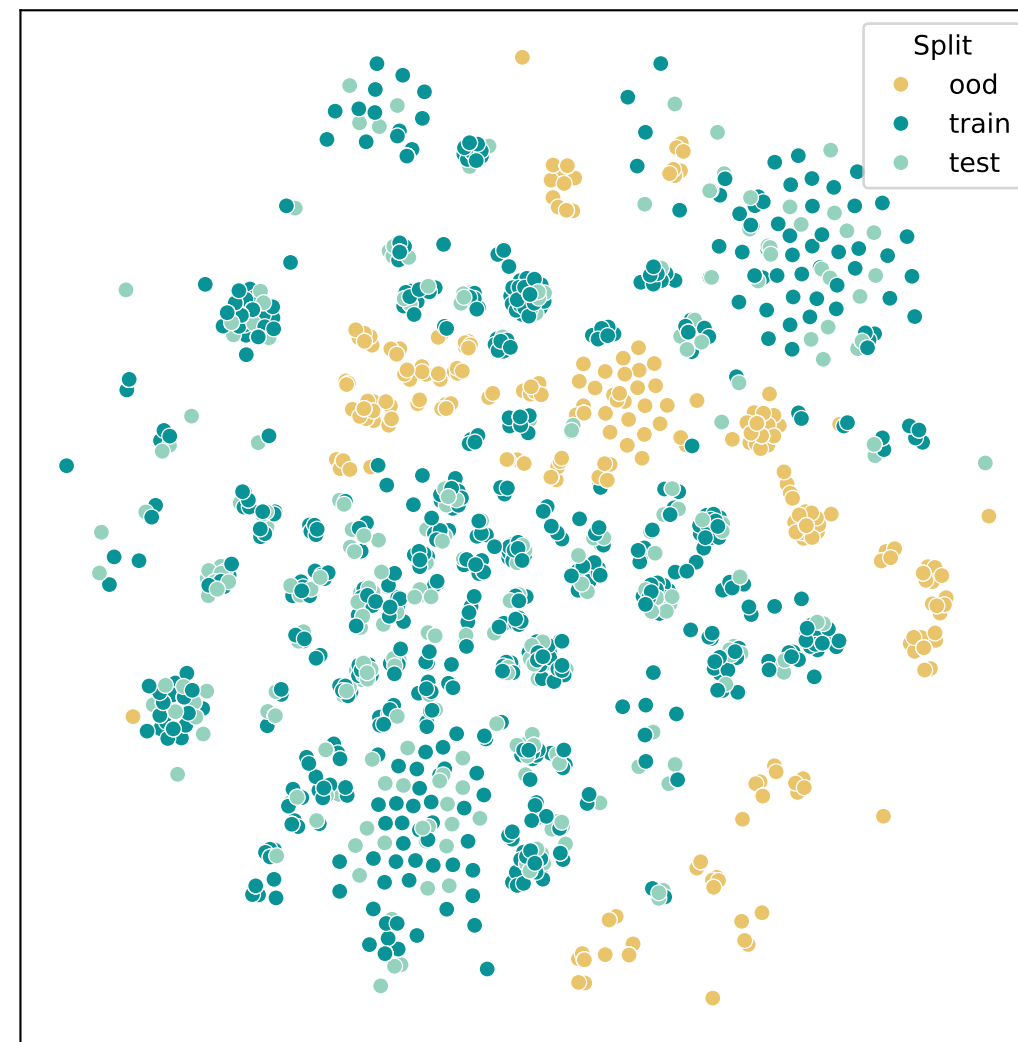


TSNE of CHEMBL236_Ki (n=2346)



Whole molecule ECFPs



Cyclic skeleton ECFPs