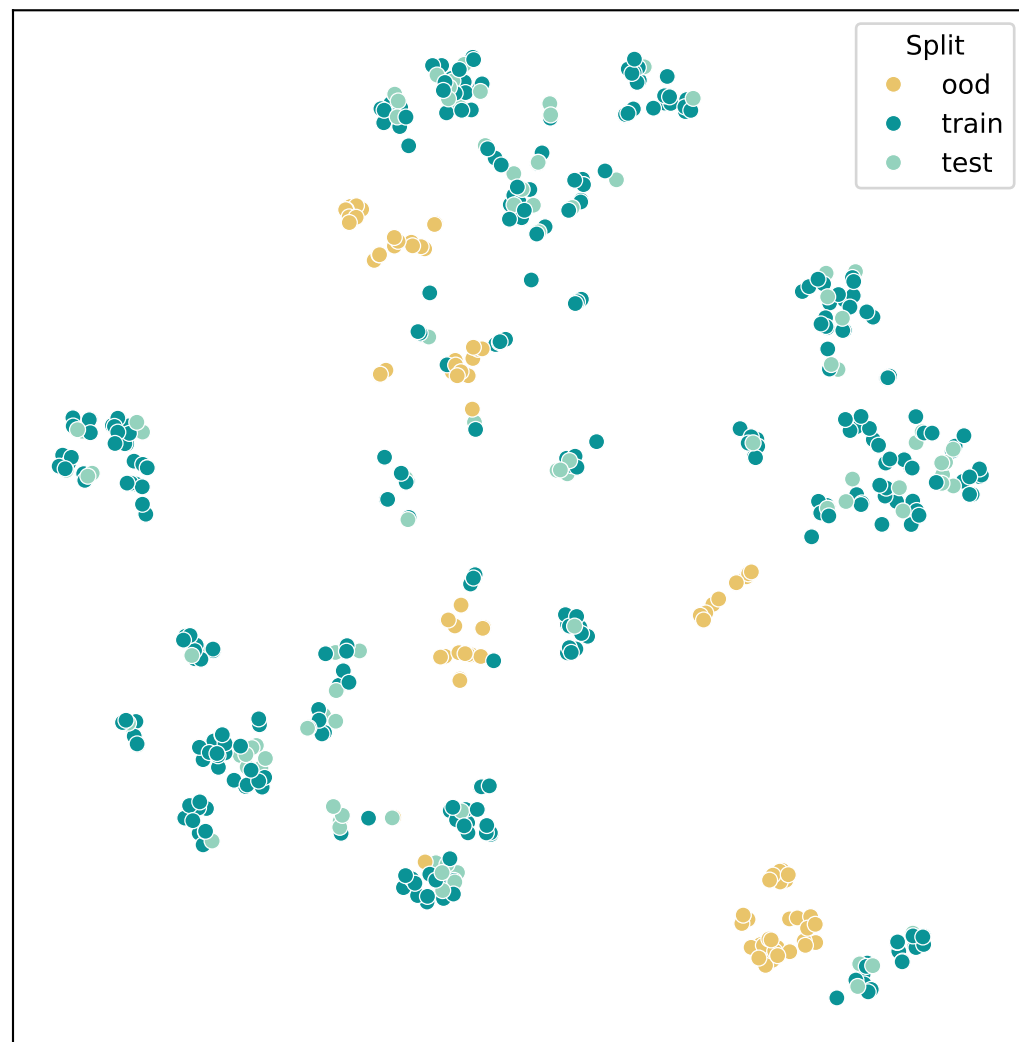
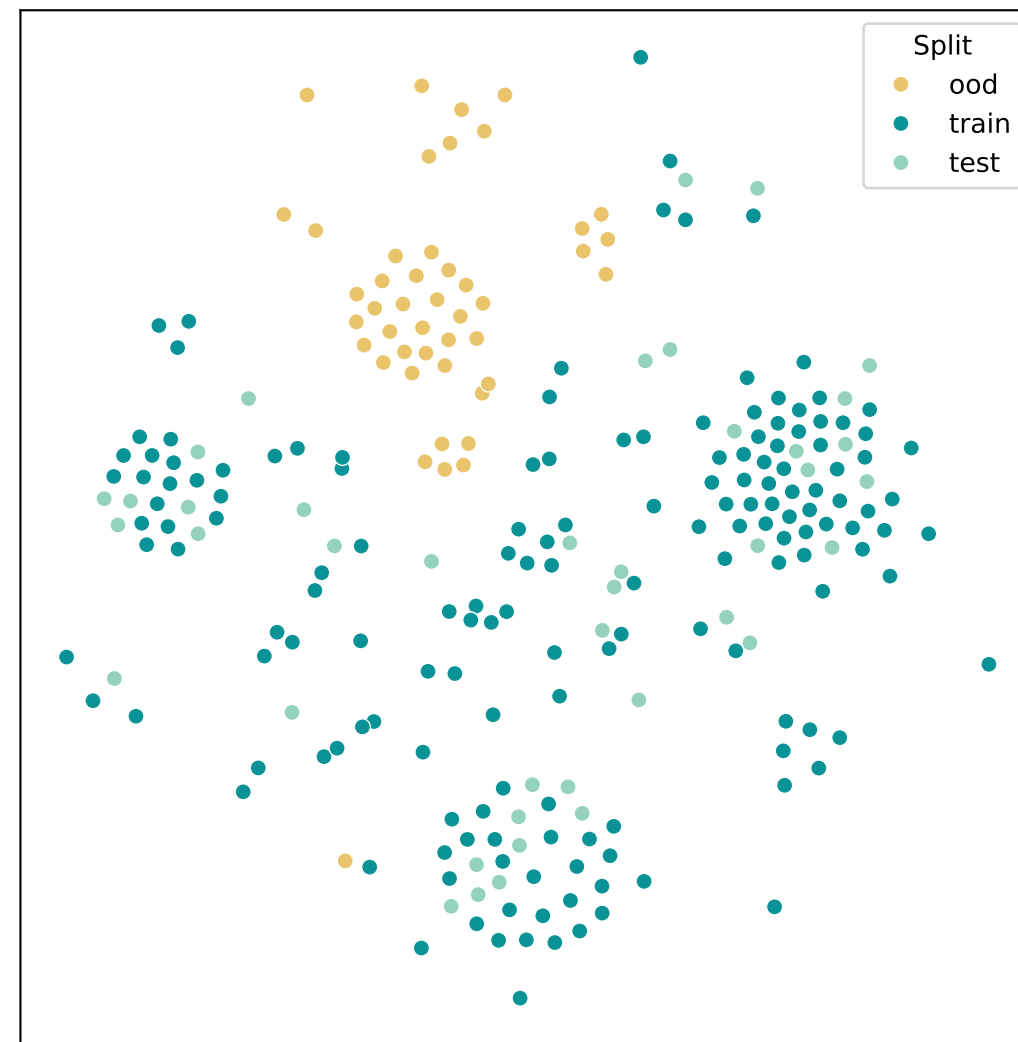


TSNE of CHEMBL1871\_Ki (n=548)



Whole molecule ECFPs



Cyclic skeleton ECFPs