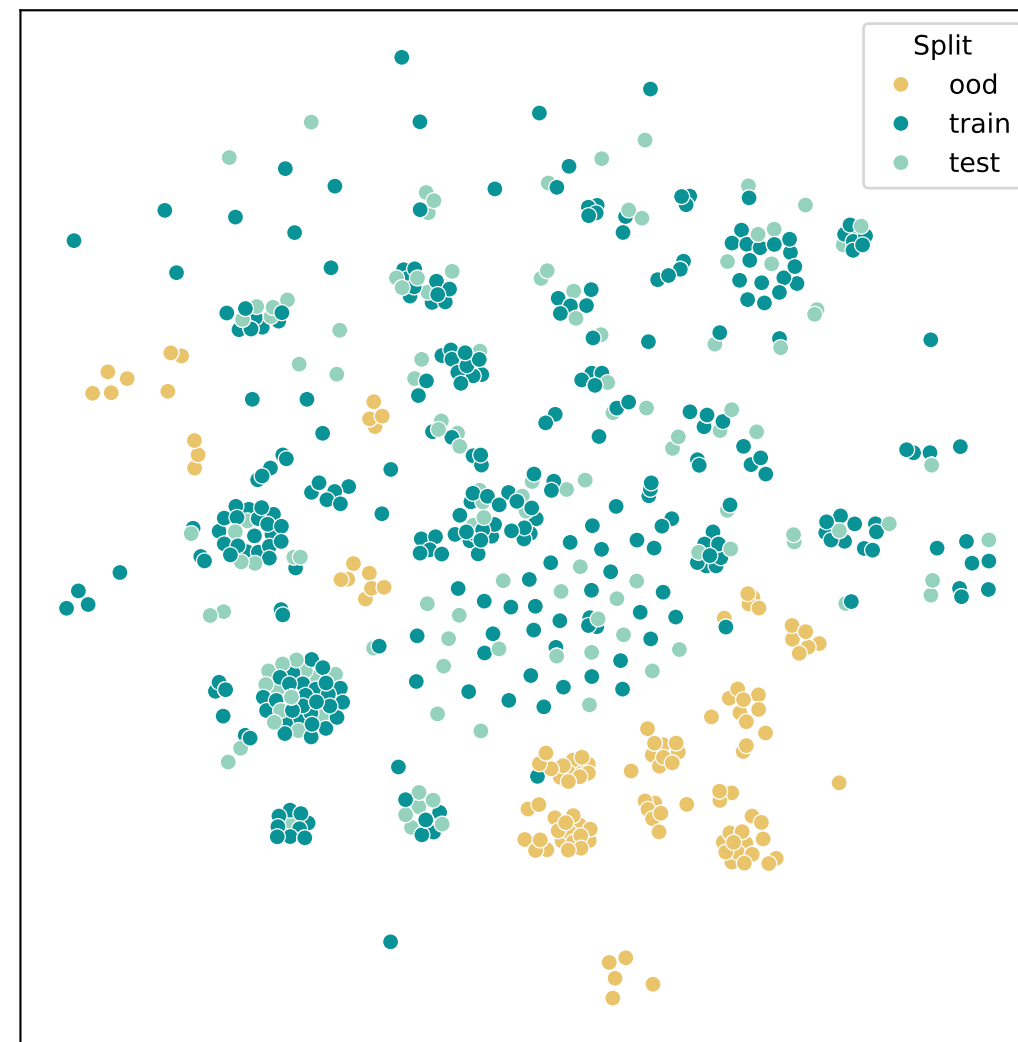


TSNE of CHEMBL231\_Ki (n=964)



Whole molecule ECFPs



Cyclic skeleton ECFPs