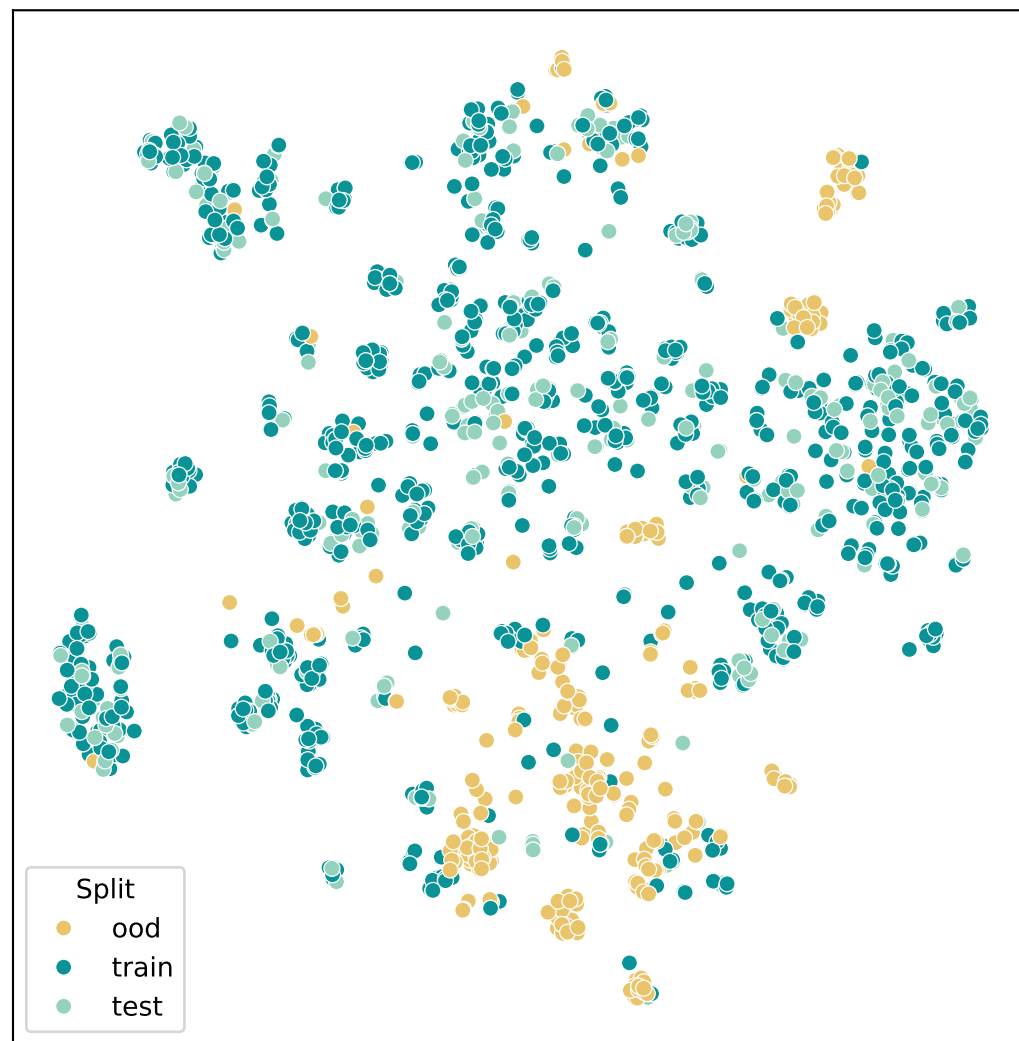
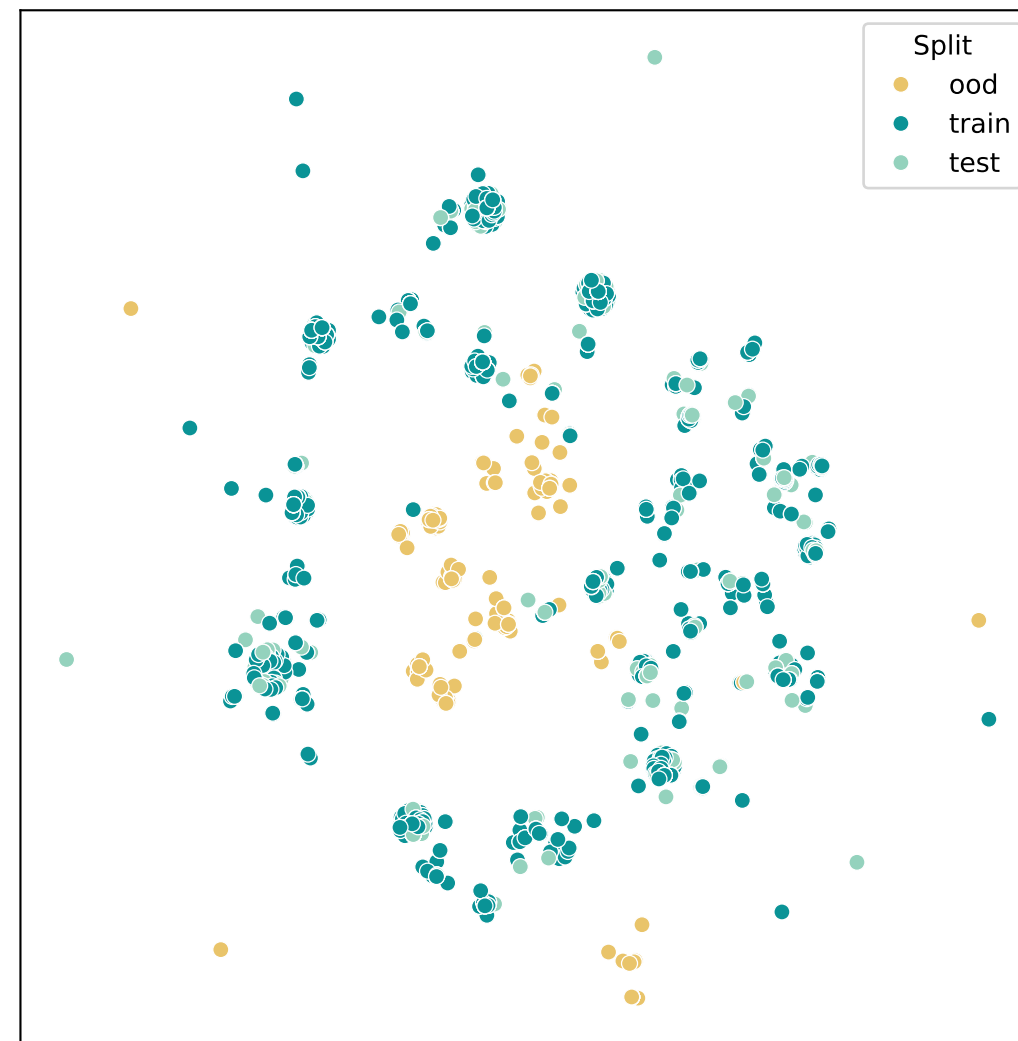


TSNE of CHEMBL219_Ki (n=1811)



Whole molecule ECFPs



Cyclic skeleton ECFPs