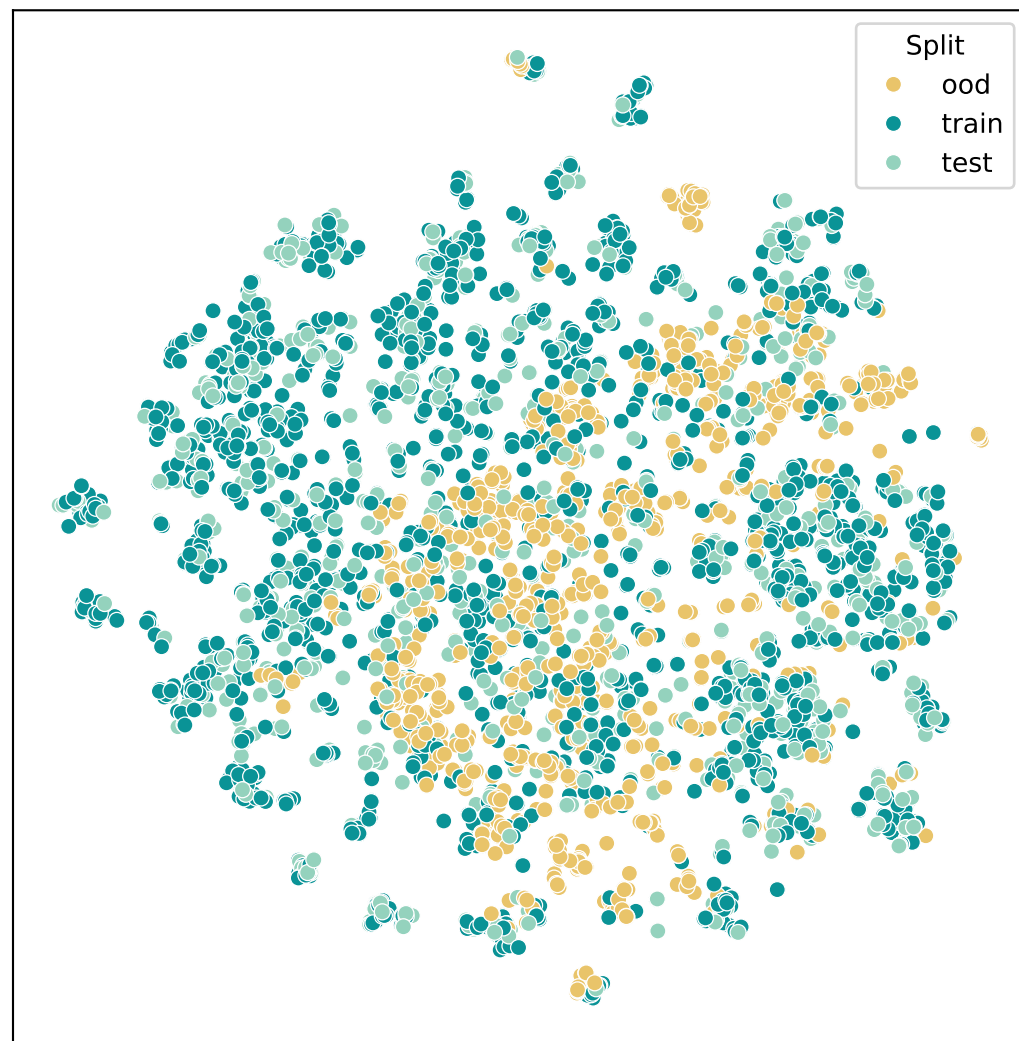
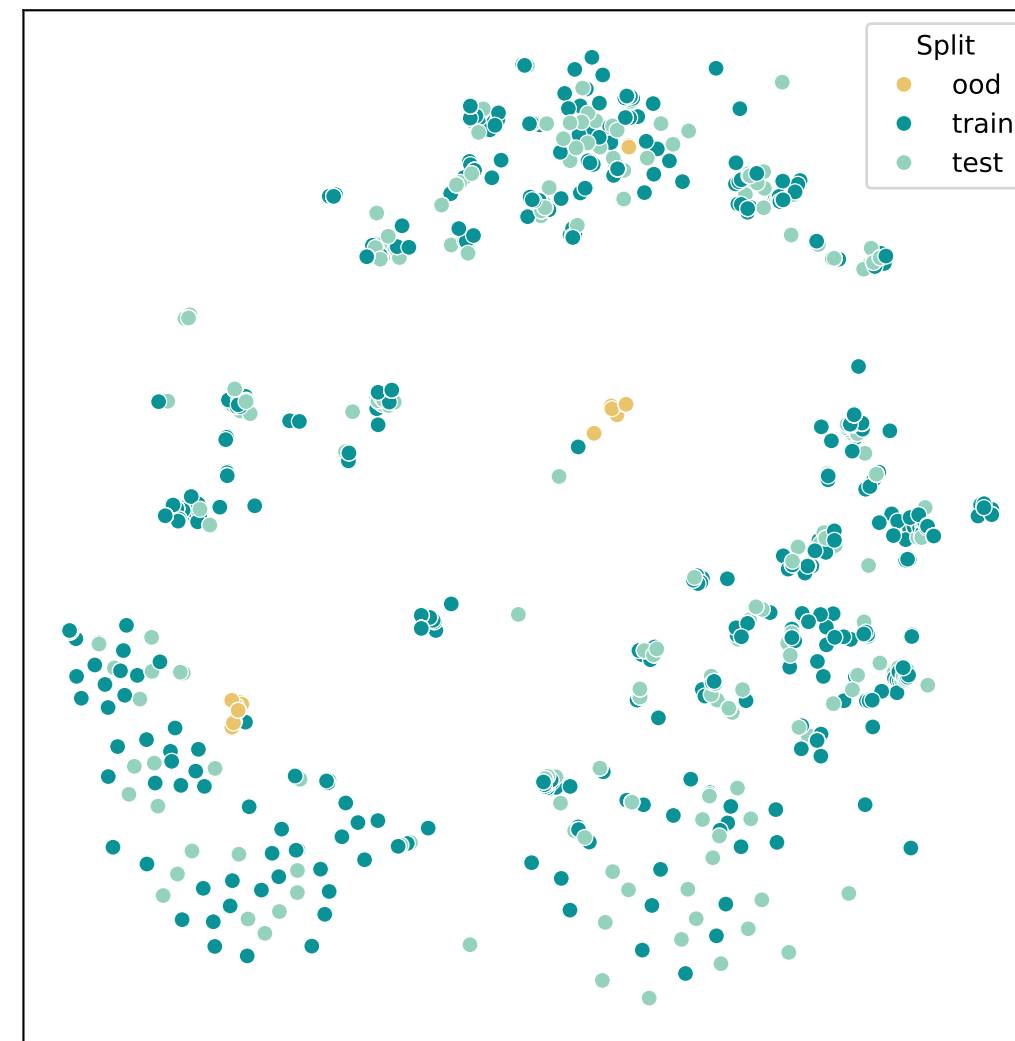


TSNE of Ames_mutagenicity (n=5125)



Whole molecule ECFPs



Cyclic skeleton ECFPs