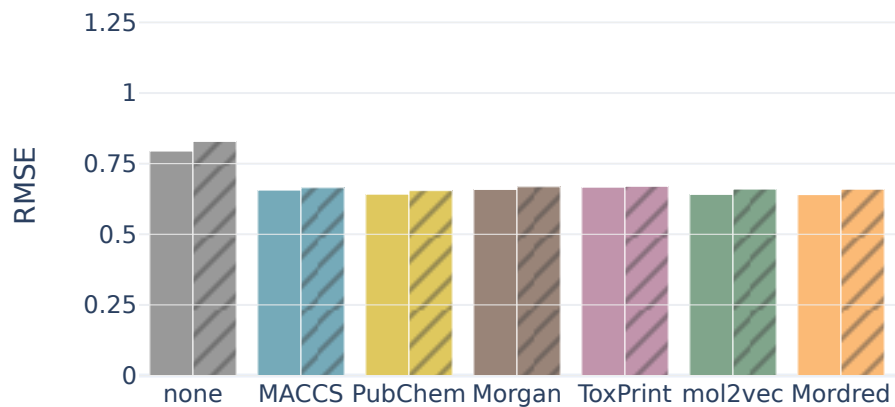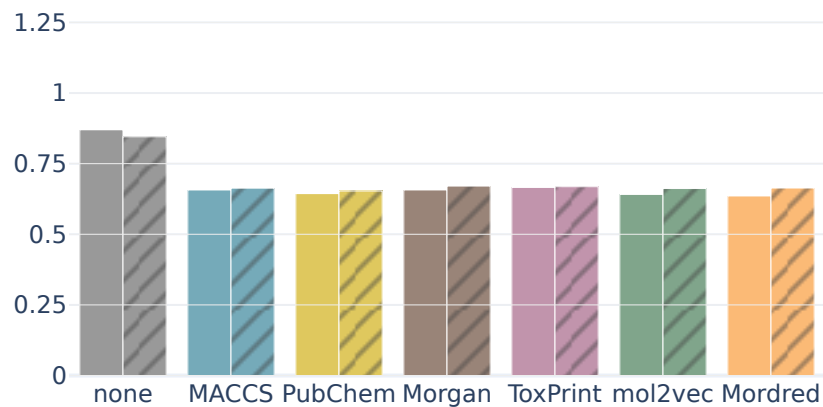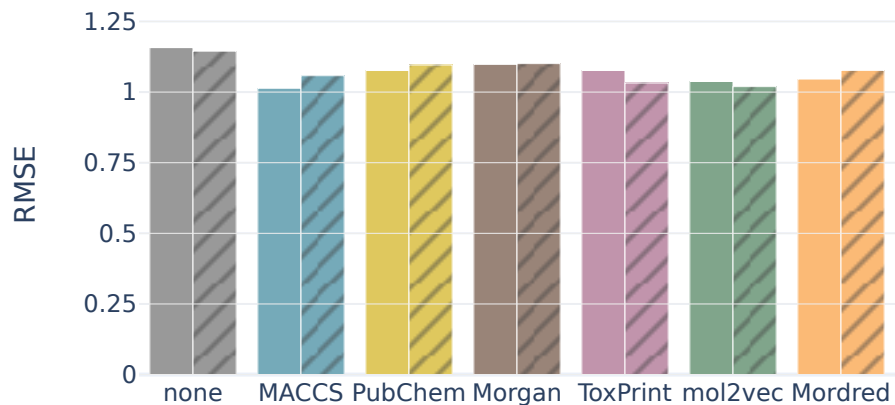totally random split
mass concentration
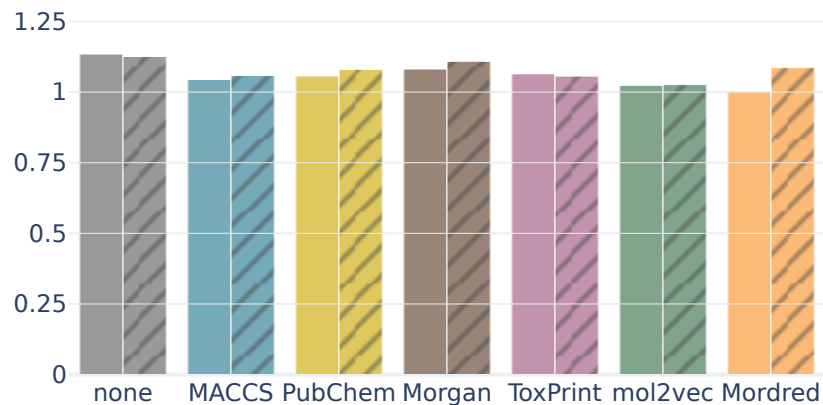
totally random split
molar concentration

split by occurrence
mass concentration

split by occurrence
molar concentration

RMSE

none MACCS PubChem Morgan ToxPrint mol2vec Mordred

pairwise distance matrix included   no   yes