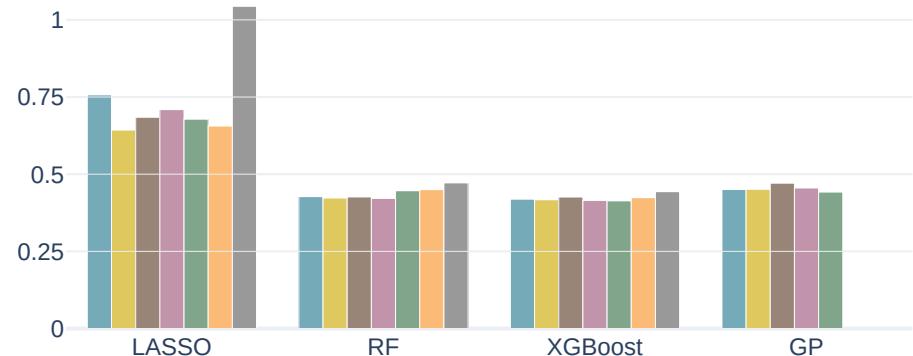


s-F2F-2

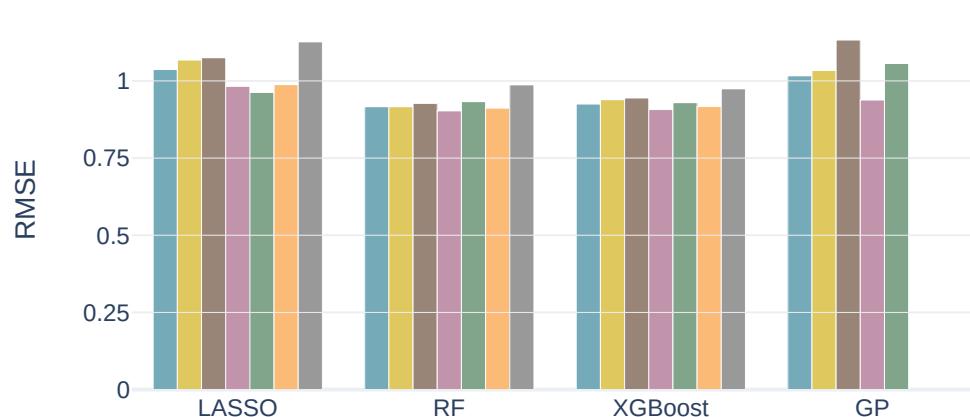
totally random split  
mass concentration



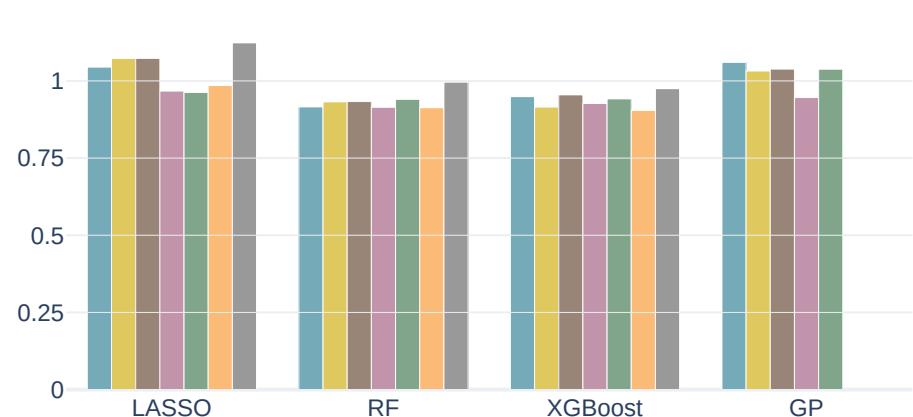
totally random split  
molar concentration



split by occurrence  
mass concentration



split by occurrence  
molar concentration



molecular representation

MACCS PubChem Morgan ToxPrint mol2vec Mordred none