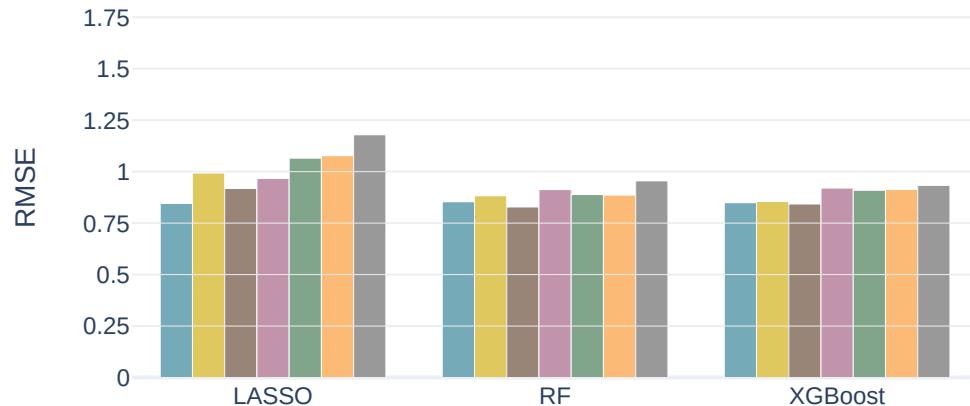
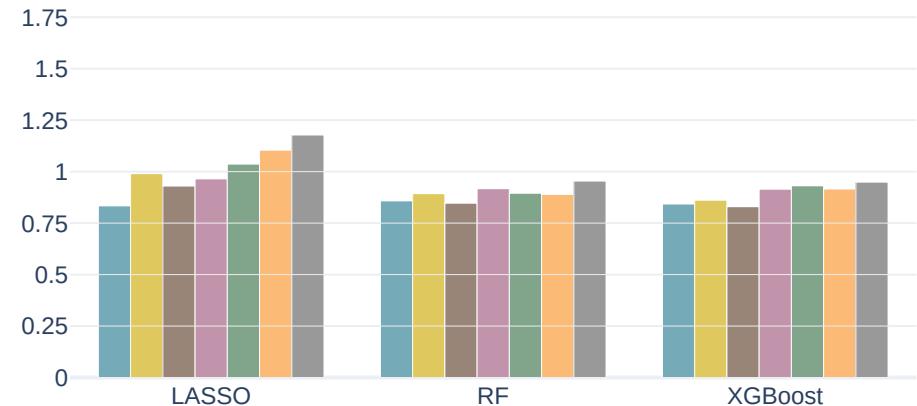


s-A2A

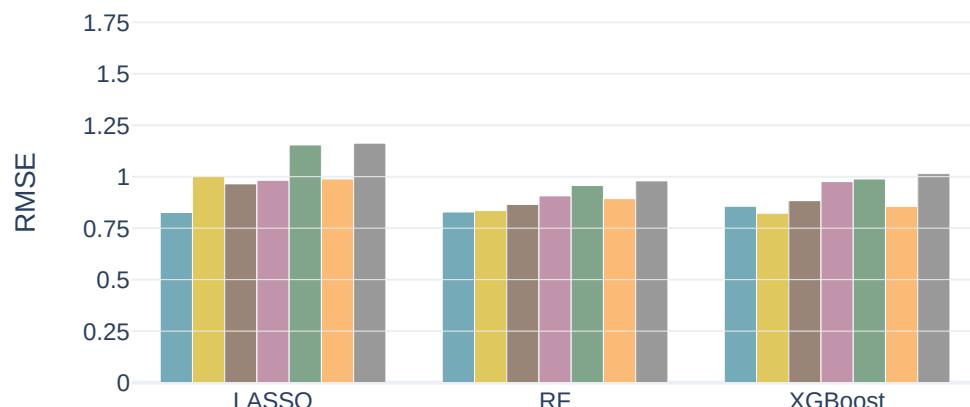
totally random split  
mass concentration



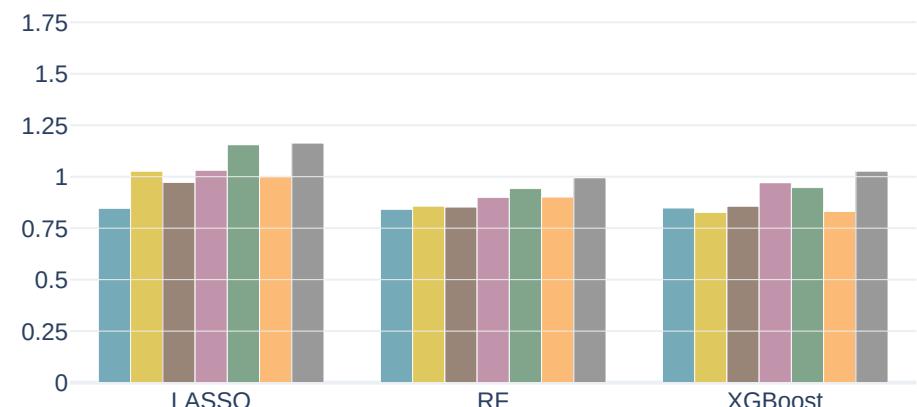
totally random split  
molar concentration



split by occurrence  
mass concentration



split by occurrence  
molar concentration



molecular representation

MACCS

PubChem

Morgan

ToxPrint

mol2vec

Mordred

none