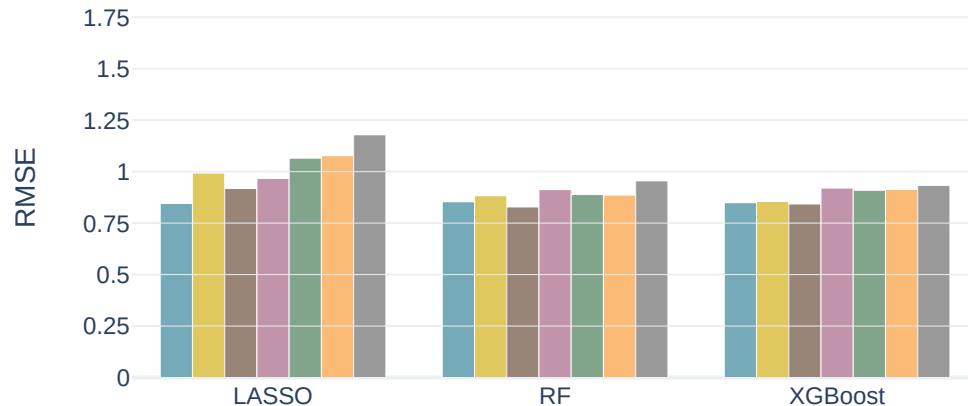
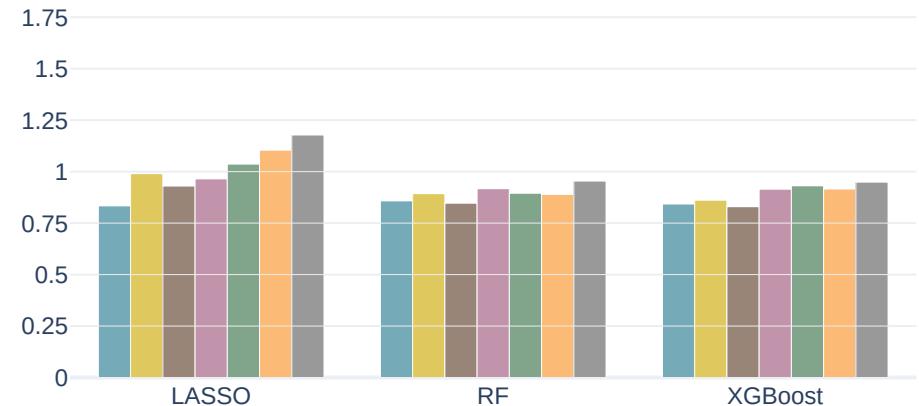


s-A2A

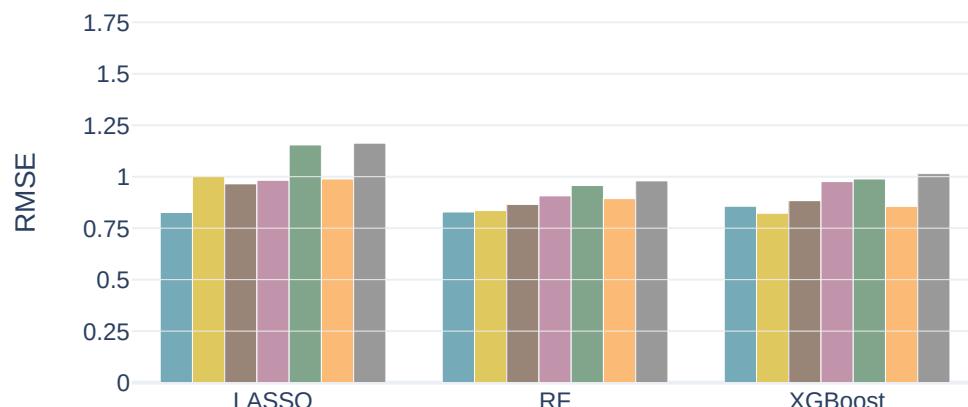
totally random split
mass concentration



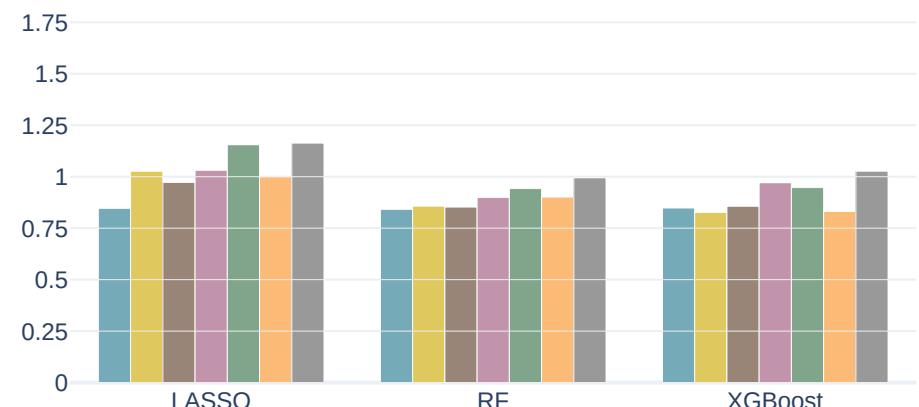
totally random split
molar concentration



split by occurrence
mass concentration



split by occurrence
molar concentration



molecular representation

MACCS

PubChem

Morgan

ToxPrint

mol2vec

Mordred

none