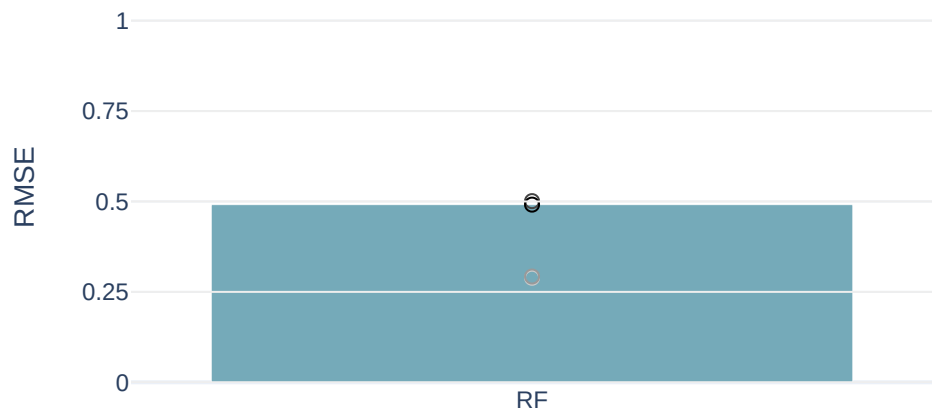
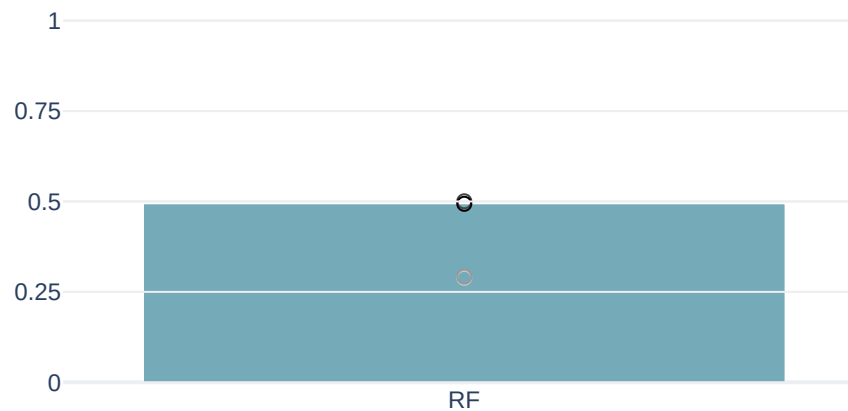


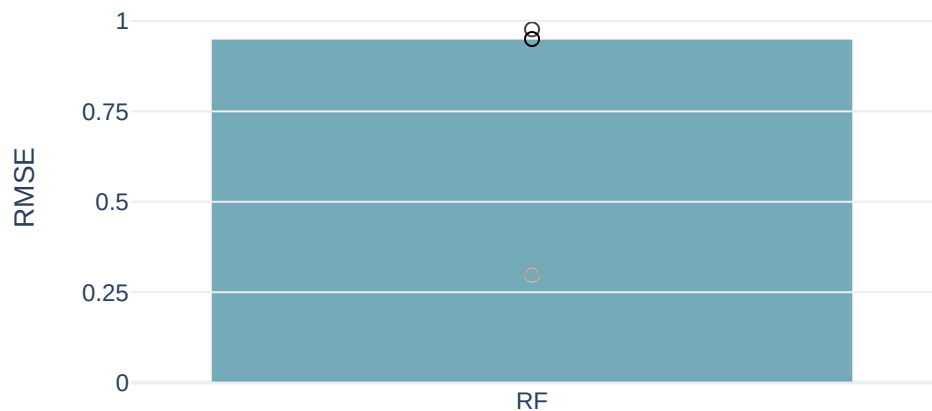
totally random split
mass concentration



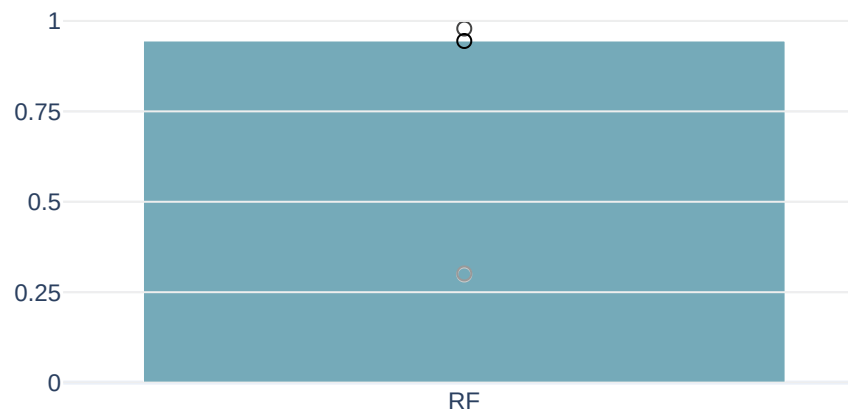
totally random split
molar concentration



split by occurrence
mass concentration



split by occurrence
molar concentration



molecular
representation

- MACCS
- PubChem
- Morgan
- ToxPrint
- mol2vec
- Mordred
- none

error type

- train
- valid
- trainvalid
- test