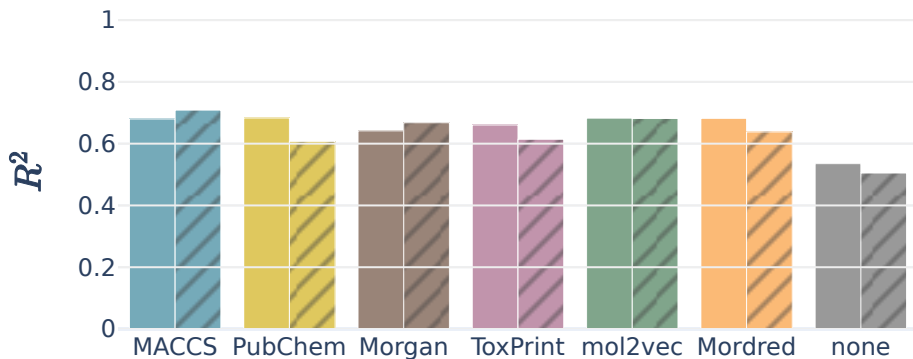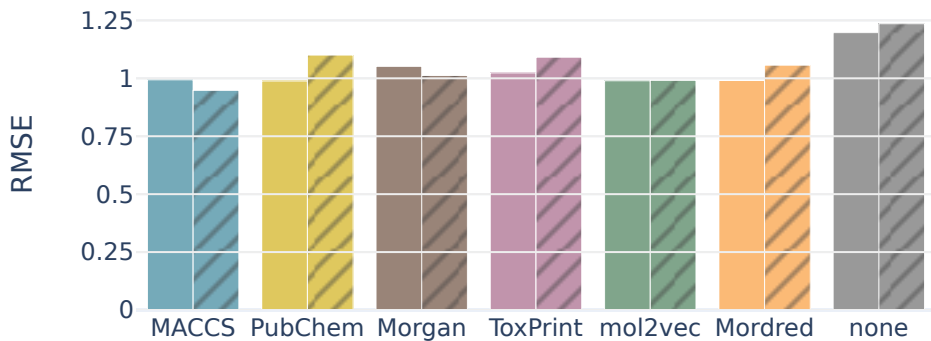split by occurrence
molar concentration

pairwise distance matrix included   no   yes