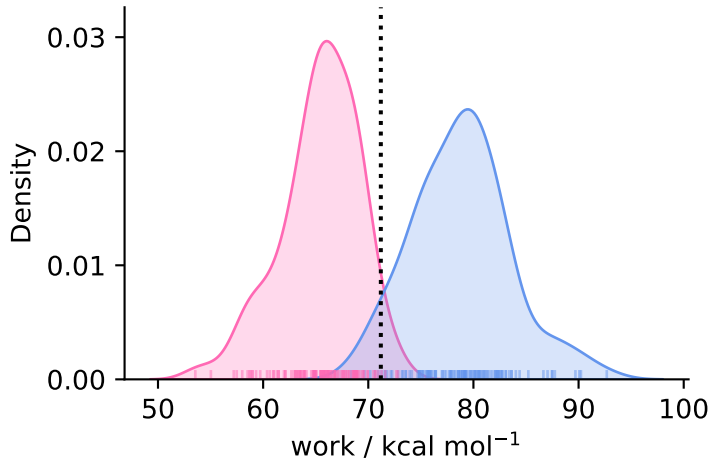RUN93

complex ($N = 118$)   solvent ($N = 100$)

direction
forward
reverse

work / kcal mol^{-1}