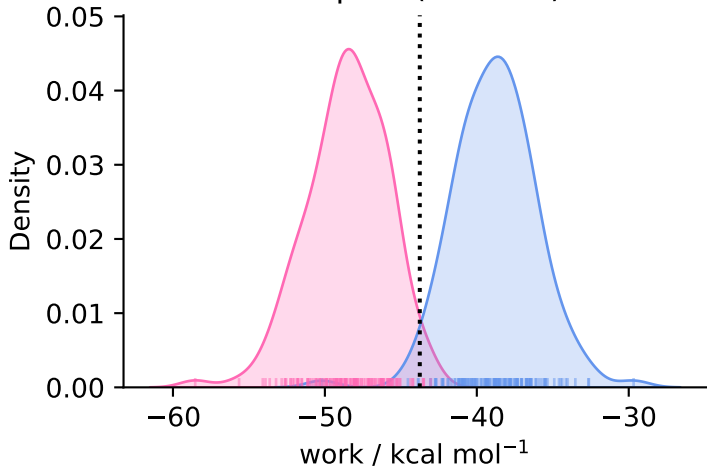RUN14044

complex ($N = 134$)

solvent ($N = 83$)

direction
forward
reverse

work / kcal mol^{-1}