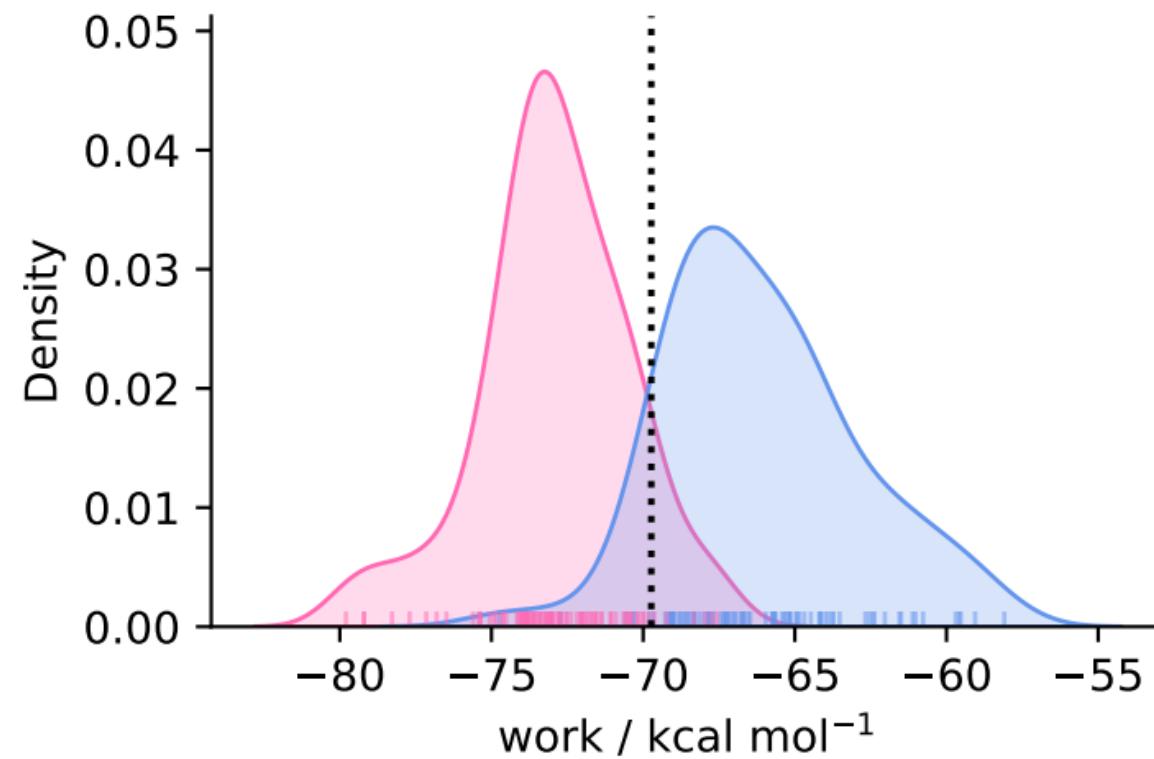RUN5740

complex ($N = 87$)   solvent ($N = 80$)

direction
forward
reverse

Density

work / kcal mol^{-1}