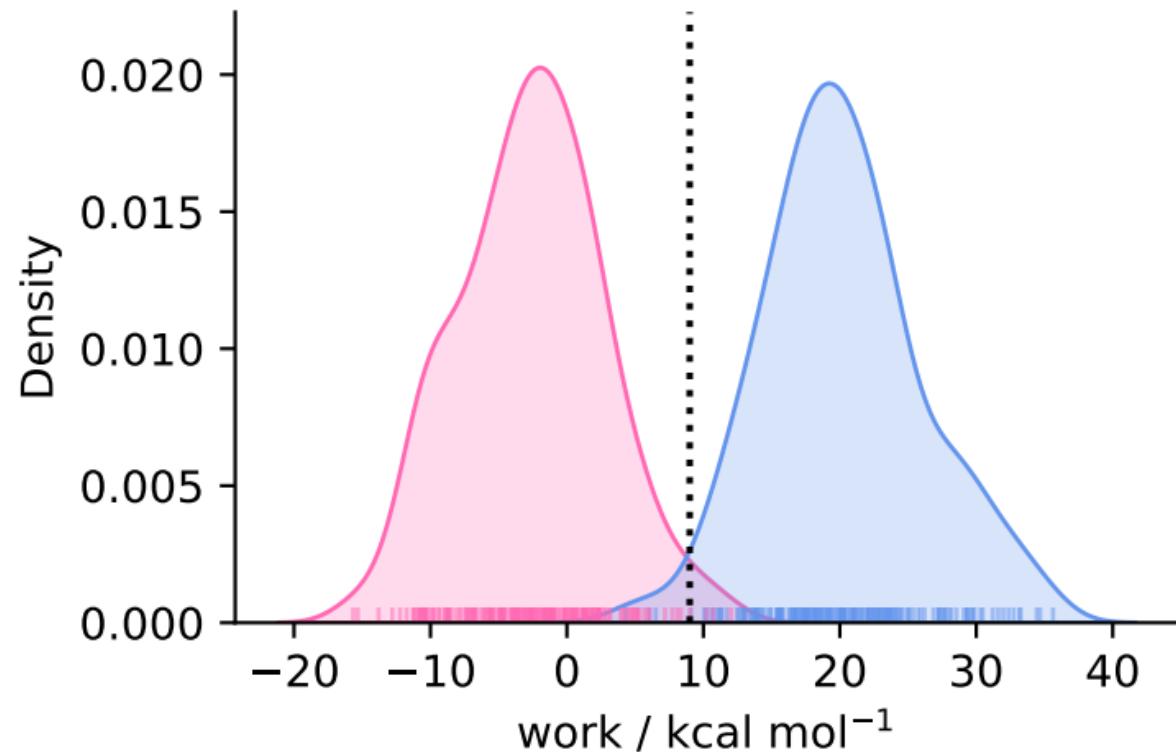RUN1559

complex ($N = 197$)

solvent ($N = 160$)

direction
forward
reverse

work / kcal mol^{-1}