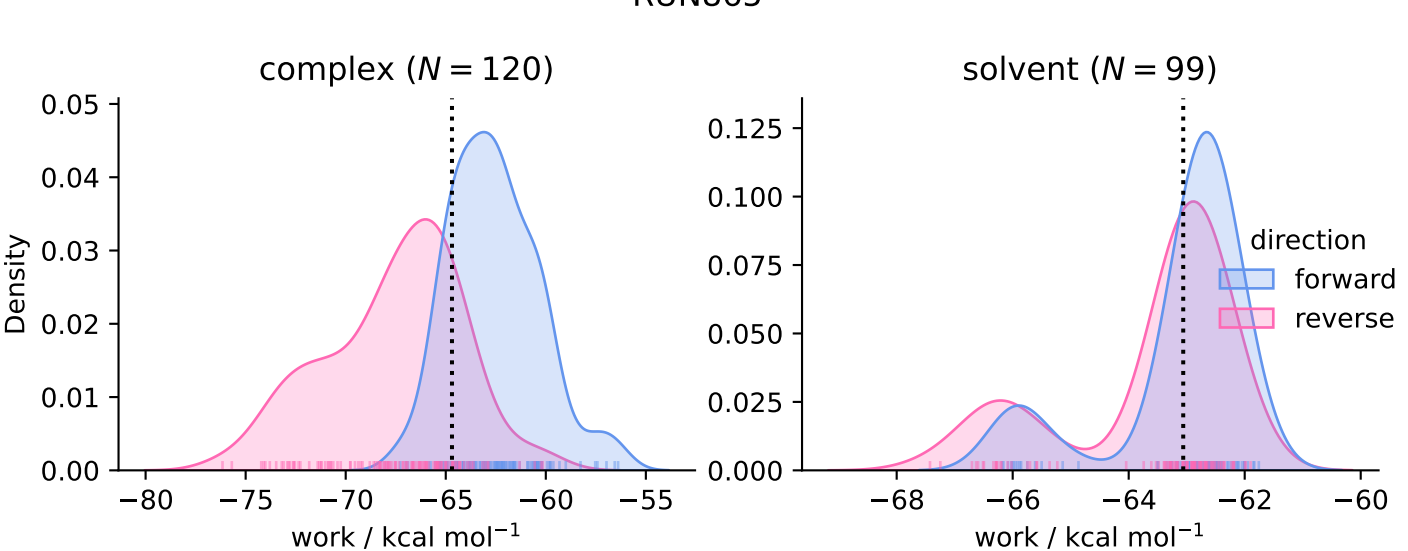
RUN865
complex ($N = 120$)
solvent ($N = 99$)
Density
0.05
0.04
0.03
0.02
0.01
0.00
0.125
0.100
0.075
0.050
0.025
0.000
−80
−75
−70
−65
−60
−55
−68
−66
−64
−62
−60
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse