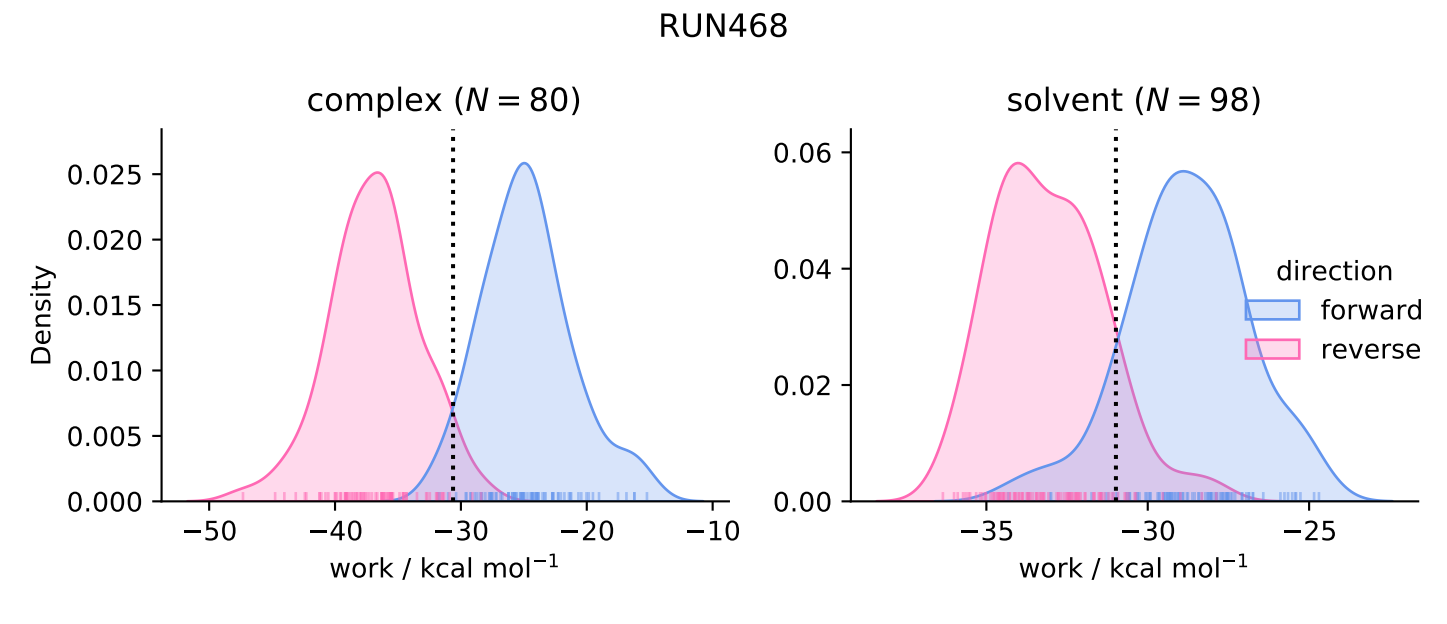
RUN468
complex ($N = 80$)
solvent ($N = 98$)
Density
0.025
0.020
0.015
0.010
0.005
0.000
0.06
0.04
0.02
0.00
−50
−40
−30
−20
−10
−35
−30
−25
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse