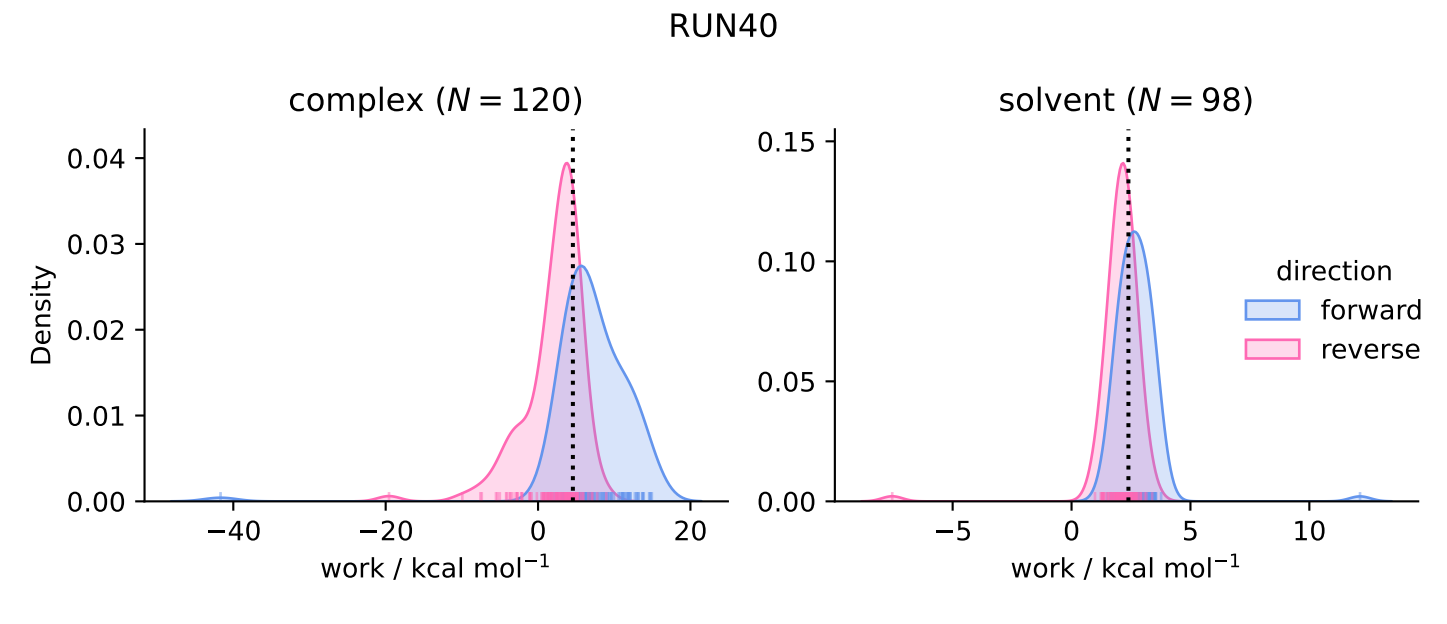
RUN40
complex ($N = 120$)
solvent ($N = 98$)
Density
0.04
0.03
0.02
0.01
0.00
0.15
0.10
0.05
−40
−20
0
20
−5
0
5
10
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse