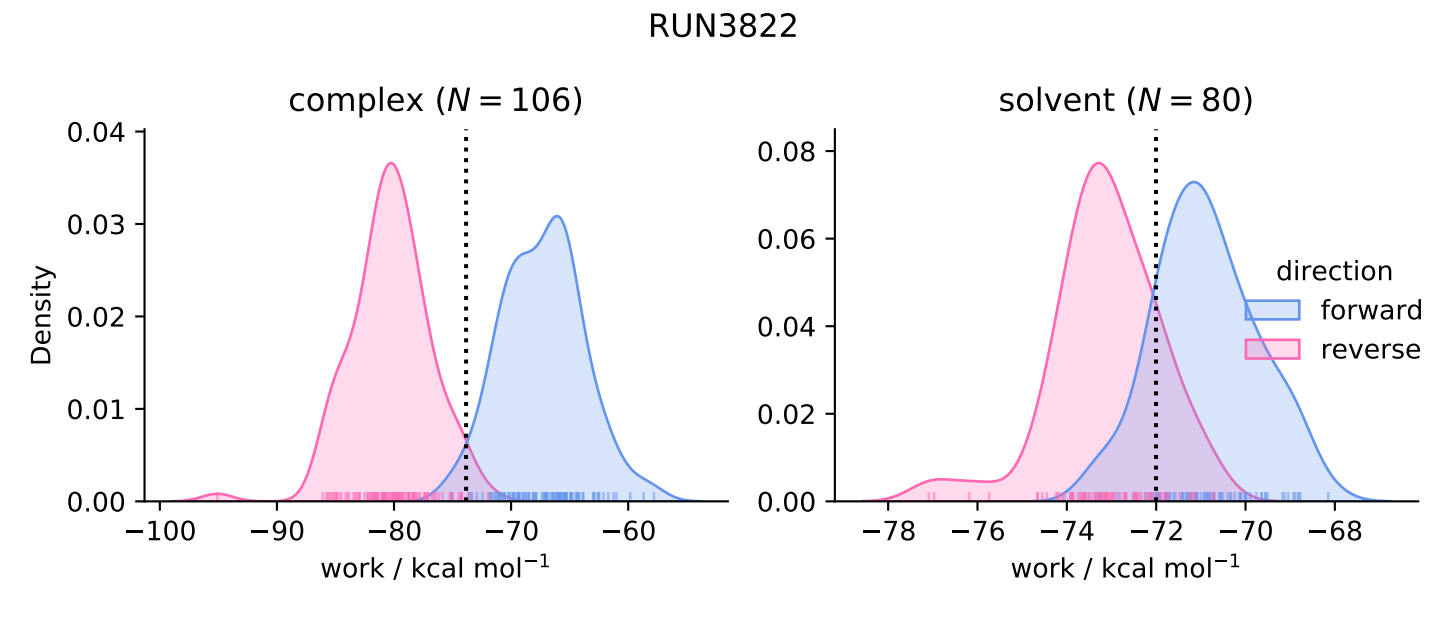
RUN3822
complex ($N = 106$)
solvent ($N = 80$)
Density
0.04
0.03
0.02
0.01
0.00
0.08
0.06
0.04
0.02
0.00
−100
−90
−80
−70
−60
−78
−76
−74
−72
−70
−68
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse