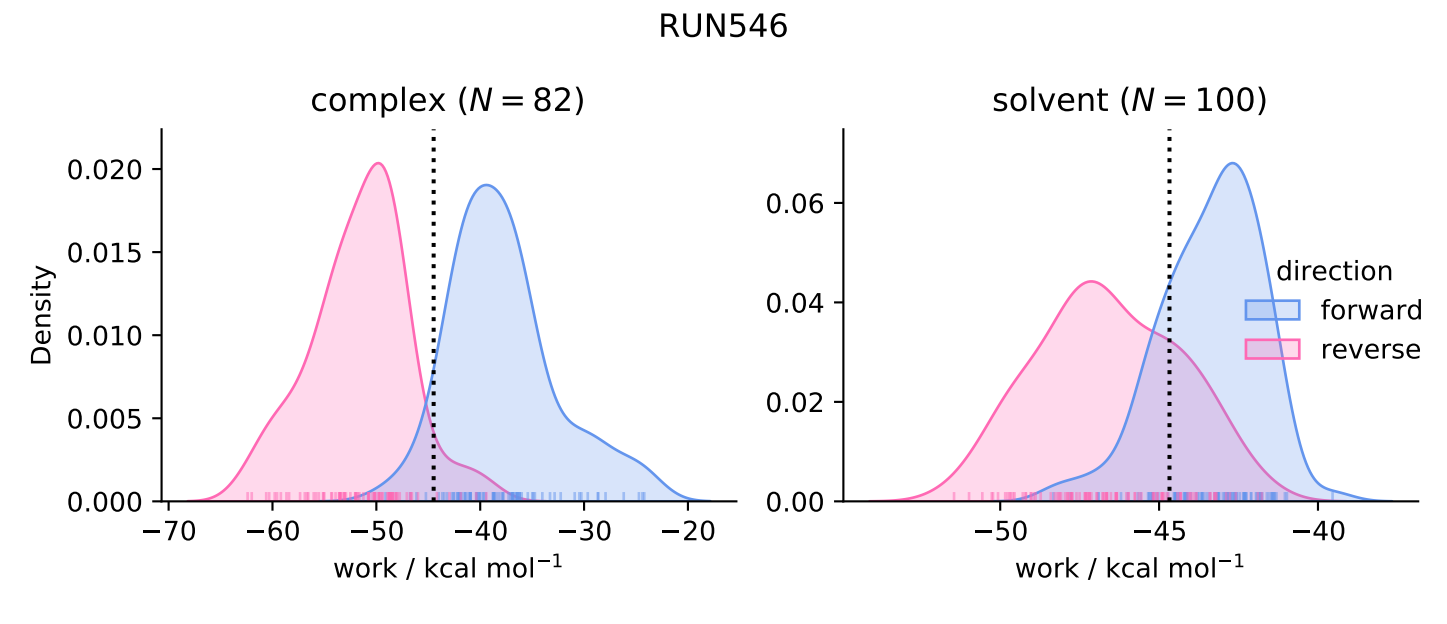
RUN546
complex ($N = 82$)
solvent ($N = 100$)
Density
0.020
0.015
0.010
0.005
0.000
0.06
0.04
0.02
0.00
−70
−60
−50
−40
−30
−20
−50
−45
−40
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse