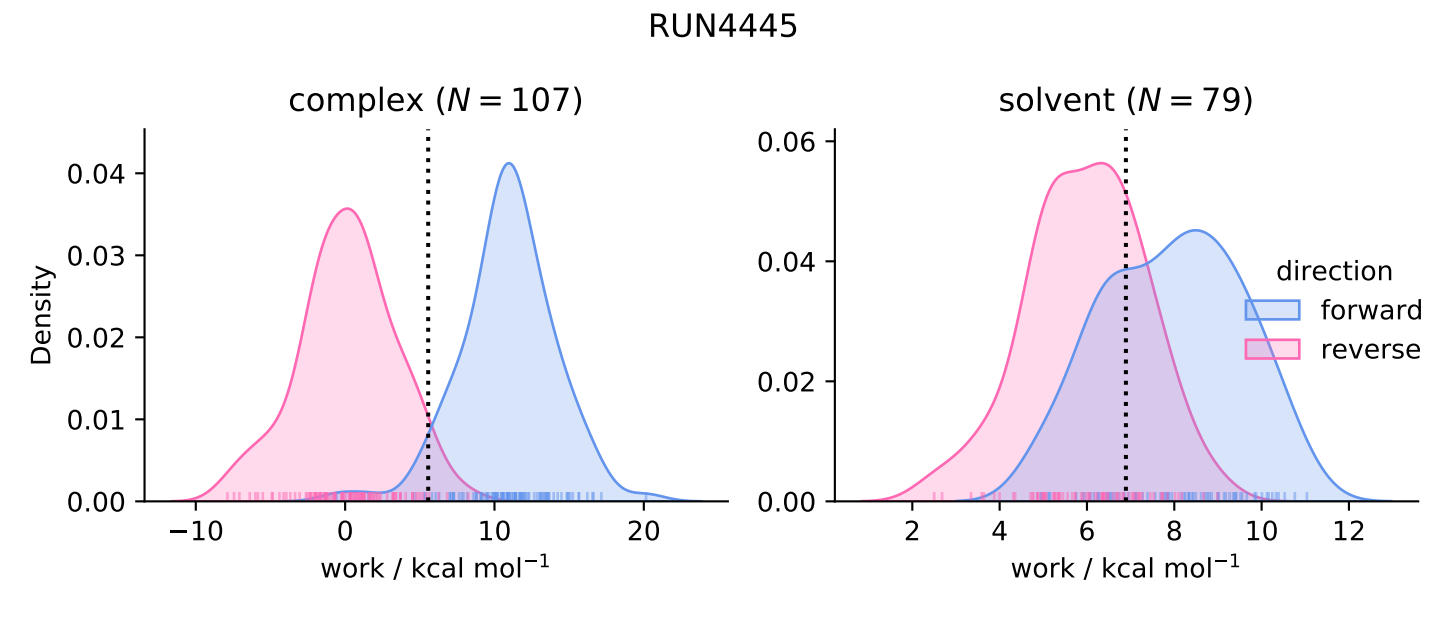
RUN4445
complex ($N = 107$)
solvent ($N = 79$)
Density
0.00
0.01
0.02
0.03
0.04
0.06
−10
0
10
20
2
4
6
8
10
12
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse