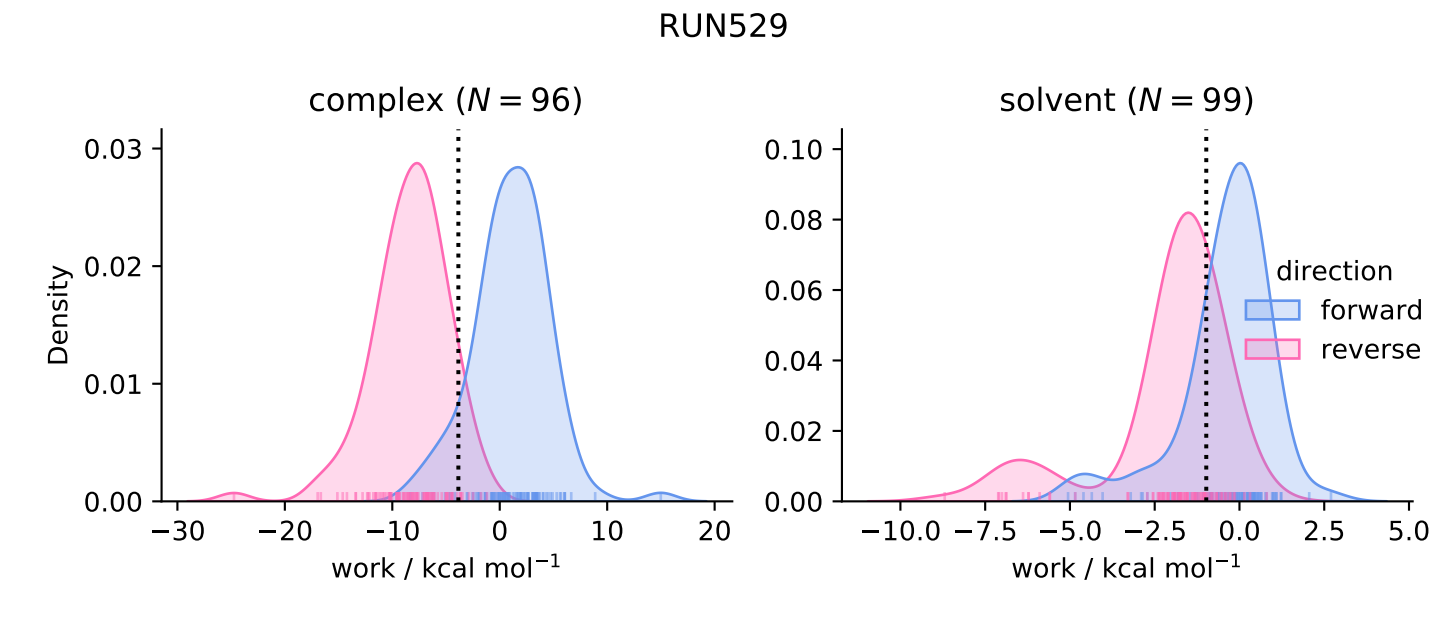
RUN529
complex ($N = 96$)
solvent ($N = 99$)
Density
0.03
0.02
0.01
0.00
0.10
0.08
0.06
0.04
0.02
0.00
−30
−20
−10
0
10
20
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse