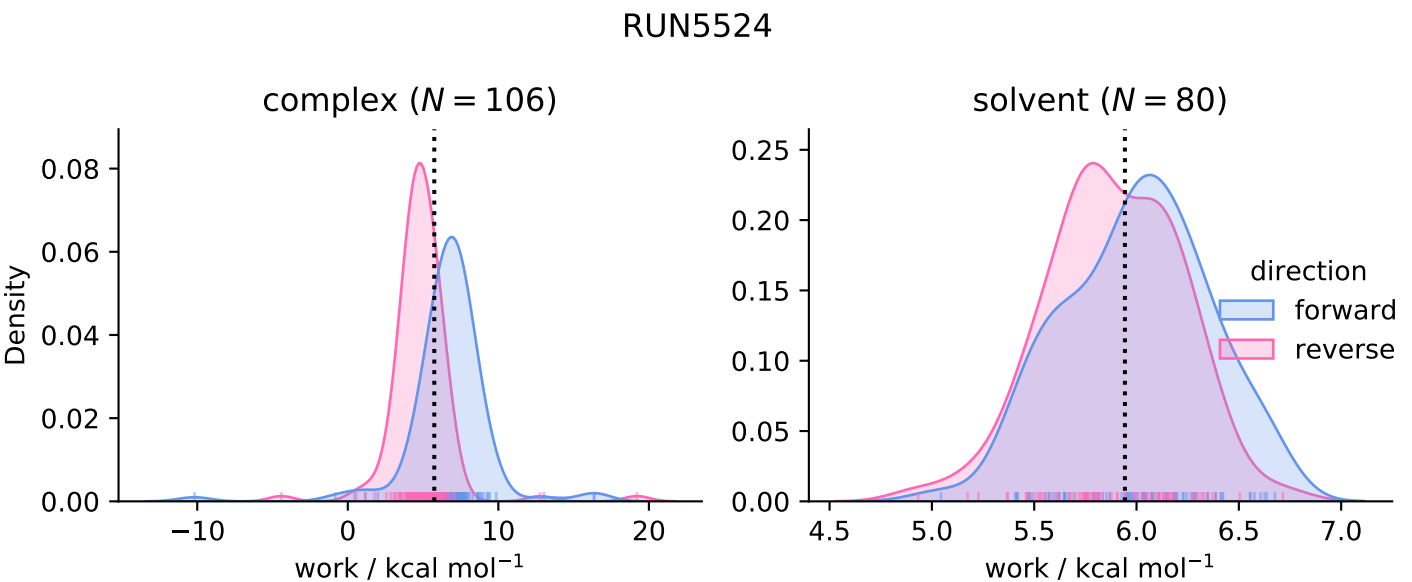
RUN5524
complex ($N = 106$)
solvent ($N = 80$)
Density
0.08
0.06
0.04
0.02
0.00
−10
0
10
20
work / kcal mol^{-1}
0.25
0.20
0.15
0.10
0.05
0.00
4.5
5.0
5.5
6.0
6.5
7.0
work / kcal mol^{-1}
direction
forward
reverse