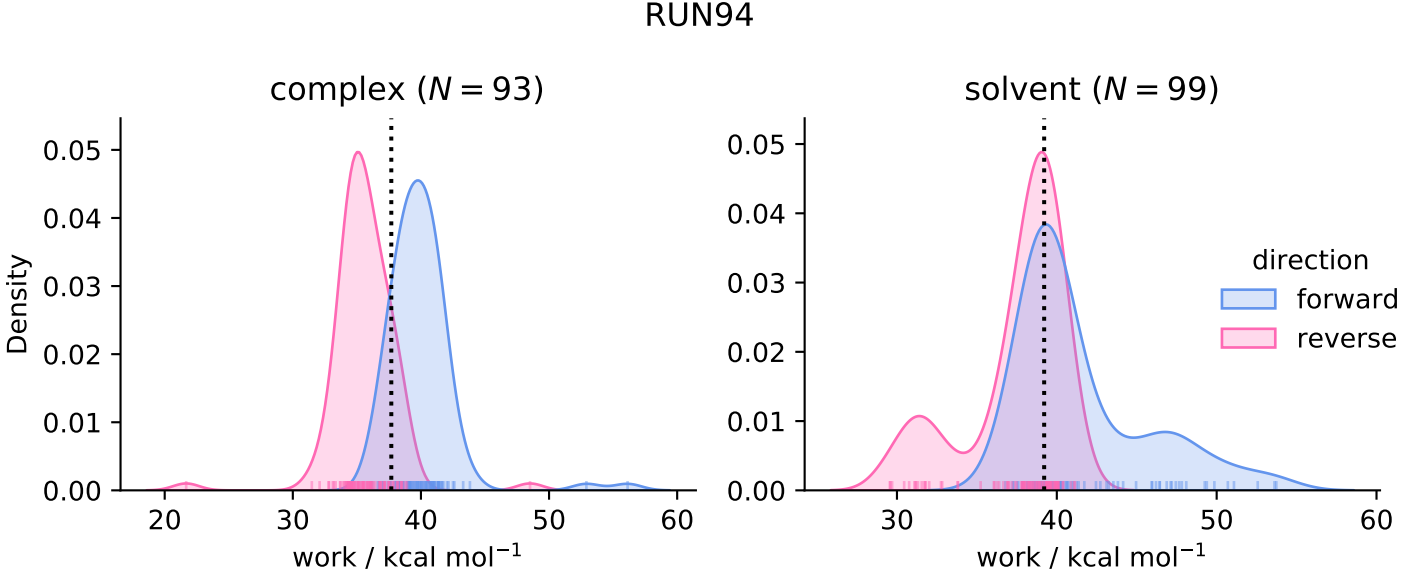
RUN94
complex ($N = 93$)
solvent ($N = 99$)
Density
0.05
0.04
0.03
0.02
0.01
0.00
20
30
40
50
60
work / kcal mol^{-1}
direction
forward
reverse