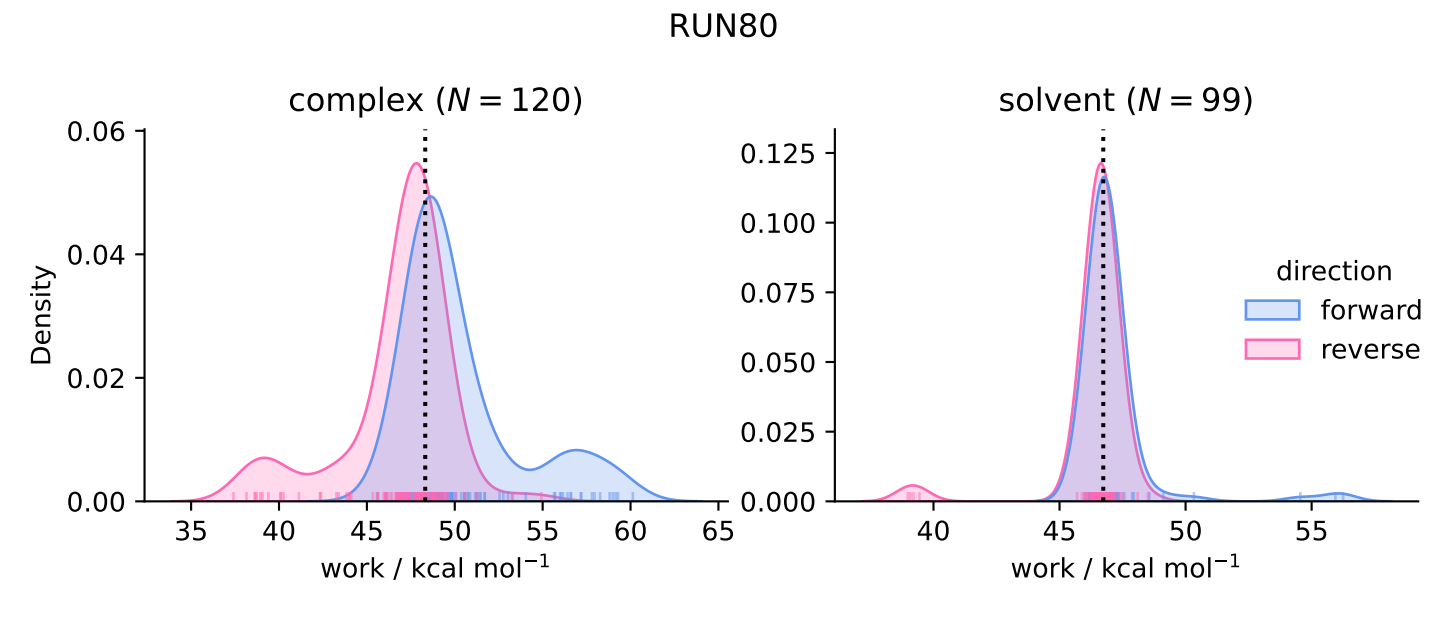
RUN80
complex ($N = 120$)
solvent ($N = 99$)
Density
0.06
0.04
0.02
0.00
0.125
0.100
0.075
0.050
0.025
0.000
35
40
45
50
55
60
65
work / kcal mol^{-1}
direction
forward
reverse