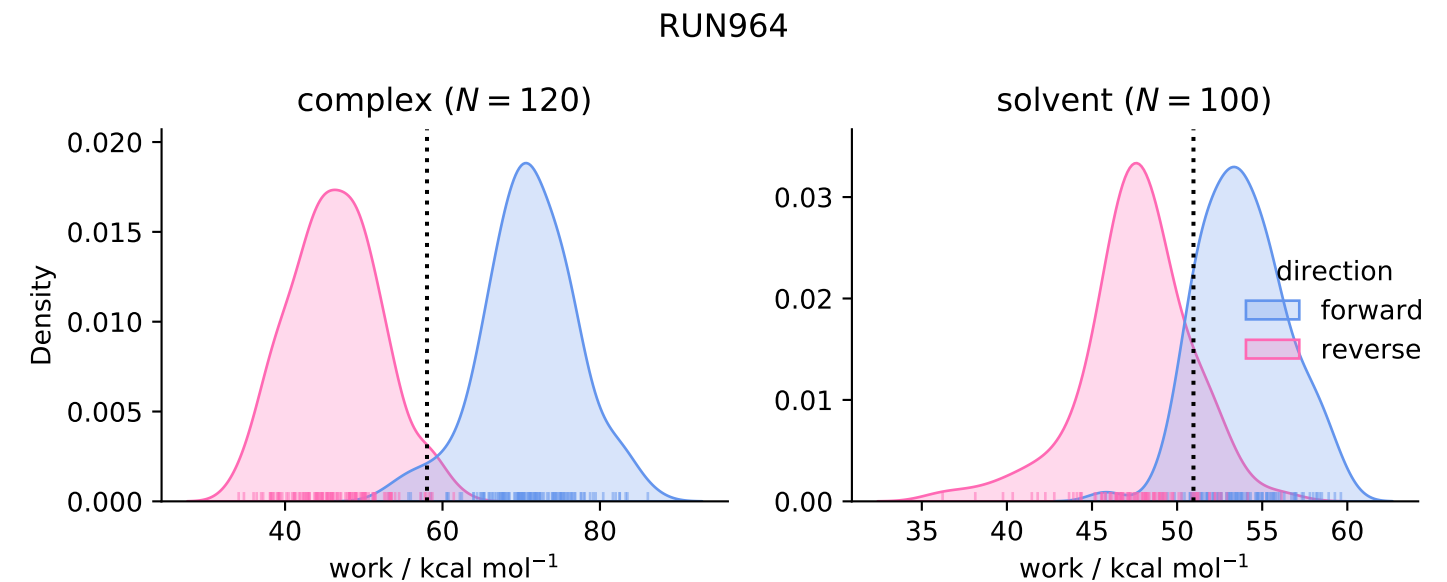
RUN964
complex ($N = 120$)
solvent ($N = 100$)
Density
0.020
0.015
0.010
0.005
0.000
0.03
0.02
0.01
0.00
40
60
80
35
40
45
50
55
60
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse