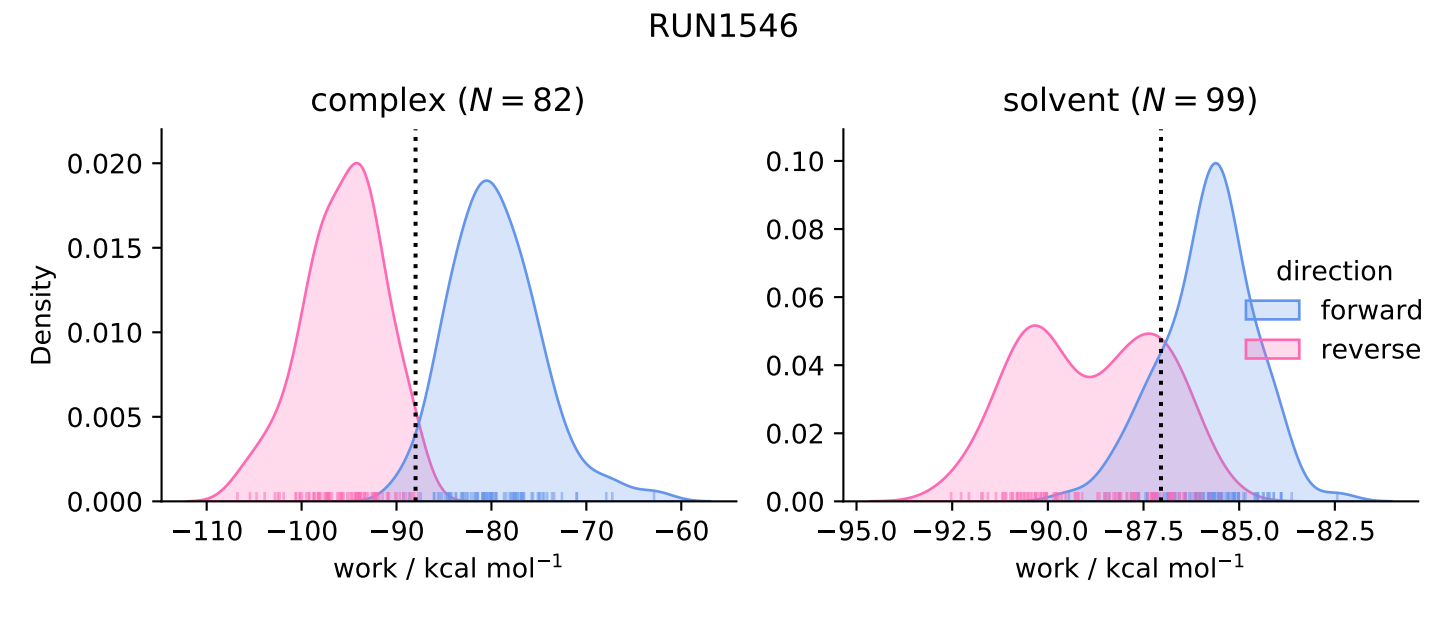
RUN1546
complex ($N = 82$)
solvent ($N = 99$)
Density
0.020
0.015
0.010
0.005
0.000
0.10
0.08
0.06
0.04
0.02
0.00
−110
−100
−90
−80
−70
−60
−95.0
−92.5
−90.0
−87.5
−85.0
−82.5
work / kcal mol^{-1}
work / kcal mol^{-1}
direction
forward
reverse