

Binding Energy of TadA*0.1-RNA Complex Using Umbrella Sampling ($k = 20 \text{ kcal/mol } \text{\AA}^2$)

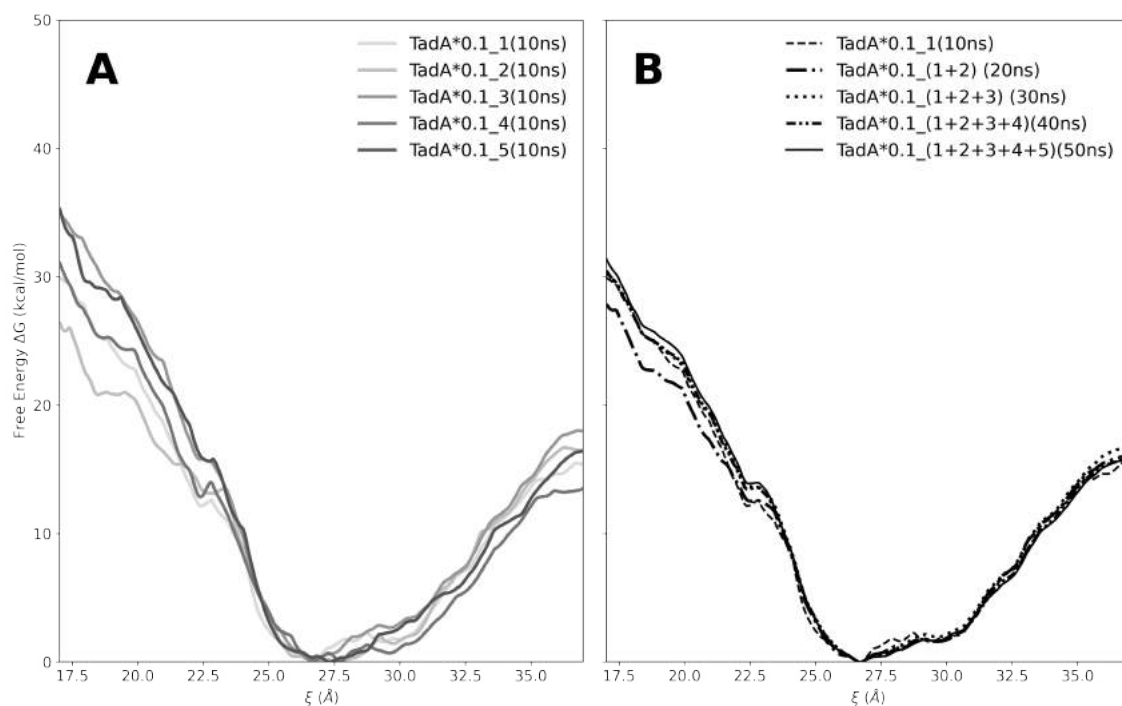


Figure S8: Analysis of the convergence for the local free energy changes in the TadA*0.1-RNA complex. (A) Free energy curves for 5 independent, 10 ns long, umbrella sampling simulations. (B) The running average of the free energy curves as these simulations are progressively combined together, from 10ns (TadA*0.1_1) to 50ns (TadA*0.1_1_2_3_4_5). This analysis shows that average free energy is converged on the time scale of umbrella sampling simulations used in this study.