

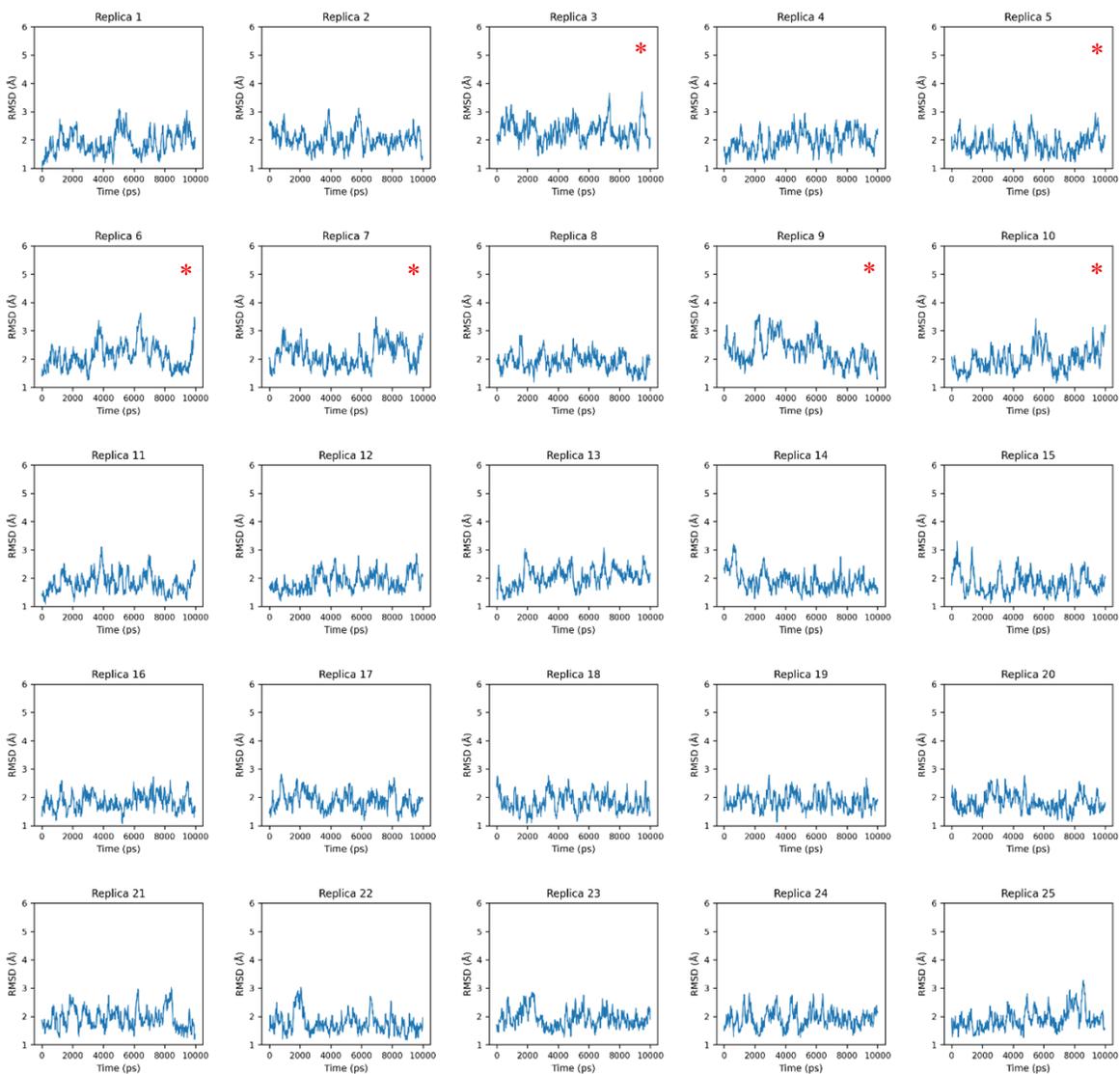
## Supplementary Information

### Ensemble Molecular Dynamics for Predicting Binding Energies of DNA Intercalators

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**Figure S1.** RMSD plots for 25 independent 10 ns MD simulation replicas of the DNA-thionine<sup>1+</sup> complex. Replicas that have relatively less stable RMSD trends are denoted with a red asterisk.