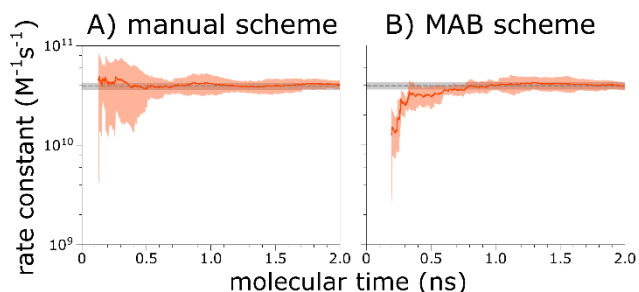


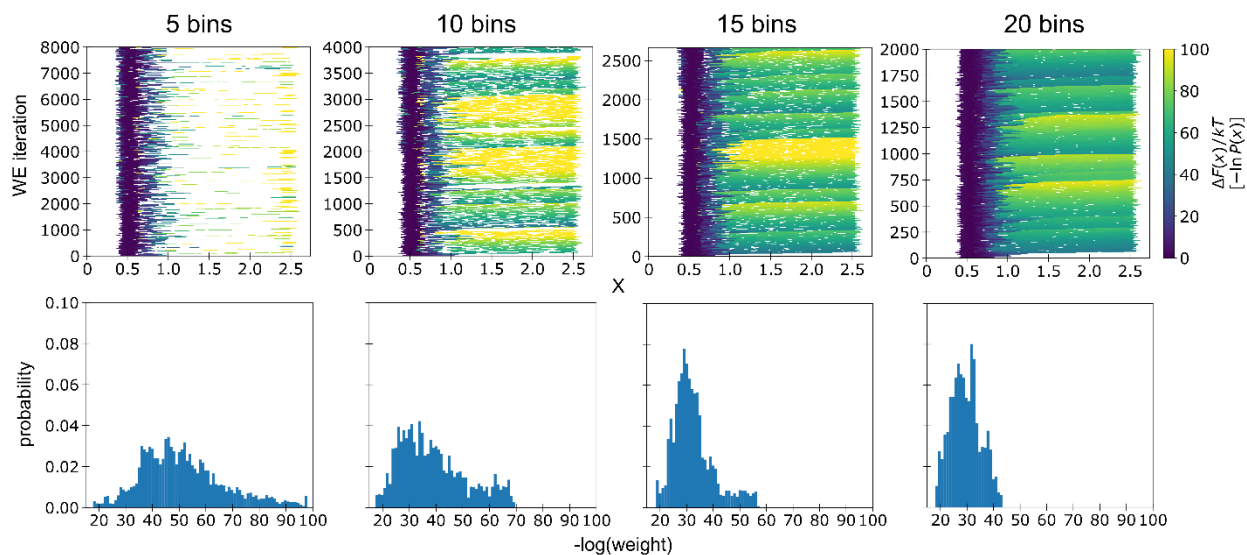
**Supporting Information for**  
**“A Minimal, Adaptive Binning Scheme for Weighted Ensemble Simulations”**

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**Figure S1. Molecular association process of Na<sup>+</sup> and Cl<sup>-</sup> ions.** Computed rate constants for the molecular association process involving Na<sup>+</sup> and Cl<sup>-</sup> ions in explicit solvent as a function of molecular time  $N\tau$  where  $N$  is the number of WE iterations and  $\tau$  is the fixed time interval for WE resampling. The rate constant from standard simulations is shown with the uncertainty as a grey shaded line. Results are shown for **A)** the manual binning scheme and **B)** the MAB scheme.



**Figure S2.** Probability distributions as a function of the progress coordinate  $X$  from WE simulations with the double-well potential and MAB scheme using different numbers of bins and the same total computing time ( $200,000 \delta t$ ). Distributions of successful trajectories by their corresponding weights (trajectory weights shown on the logscale) are shown in the second row.