Interaction of Hoechst 33342 with POPC membranes at different pH values

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Supplemental Figures

Contents

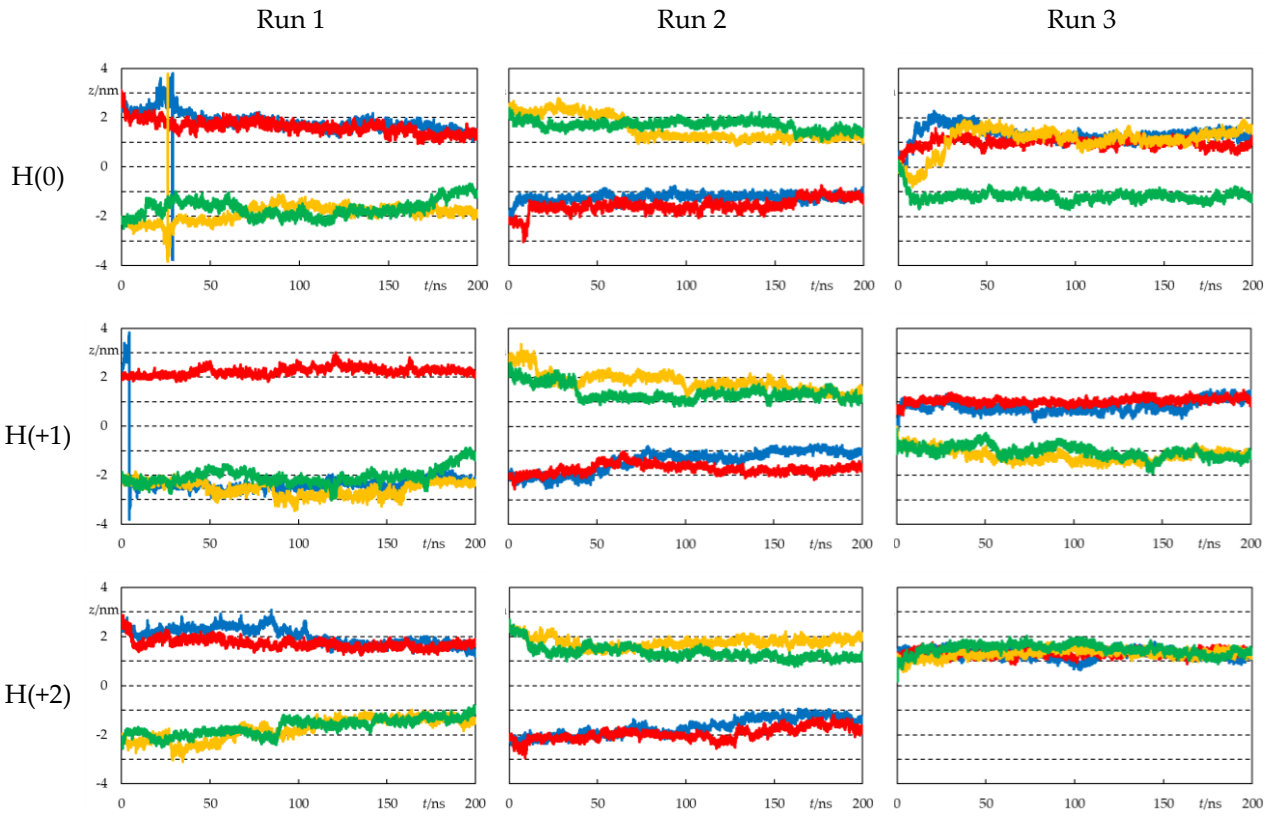

Figure S1. Time variations of the center of mass positions along the bilayer normal, respective to the that of the bilayer center of mass (z = 0), of all four individual molecules in each simulation. Discontinuities in runs 1 of H(0) and H(+1) indicate molecules that diffused through the water medium, crossed the vertical limit of the box and reappeared on the opposite side.

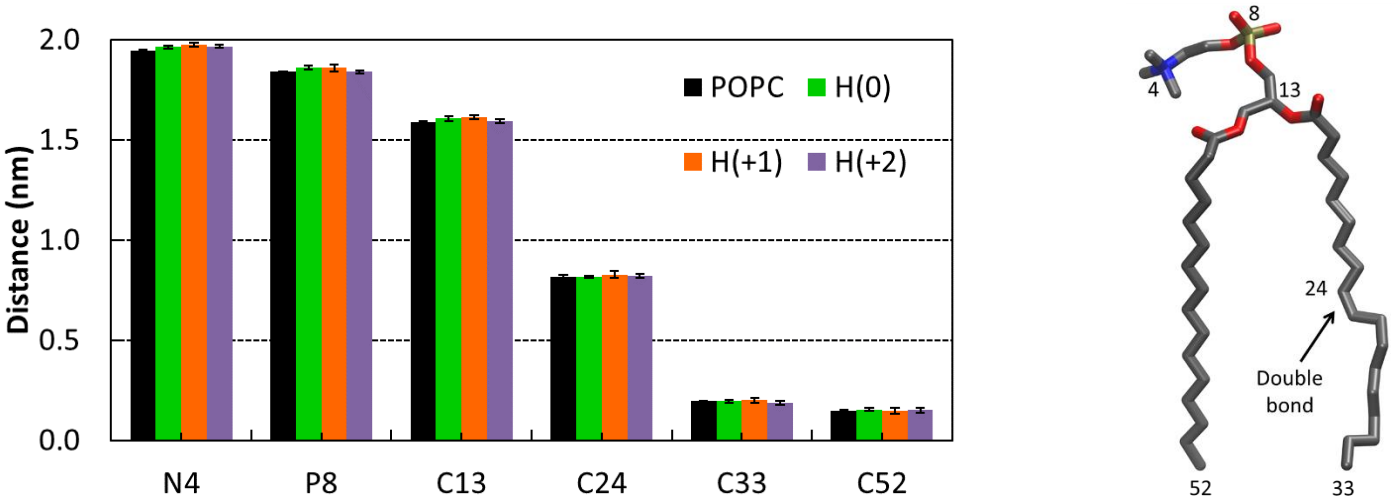

Figure S2. Average transverse distances to the bilayer center for selected atoms of POPC (numbering defined in the structure on the right), for systems without probe (POPC) and in the presence of H33342 in different ionization states (H(0), H(+1) and H(+2)).

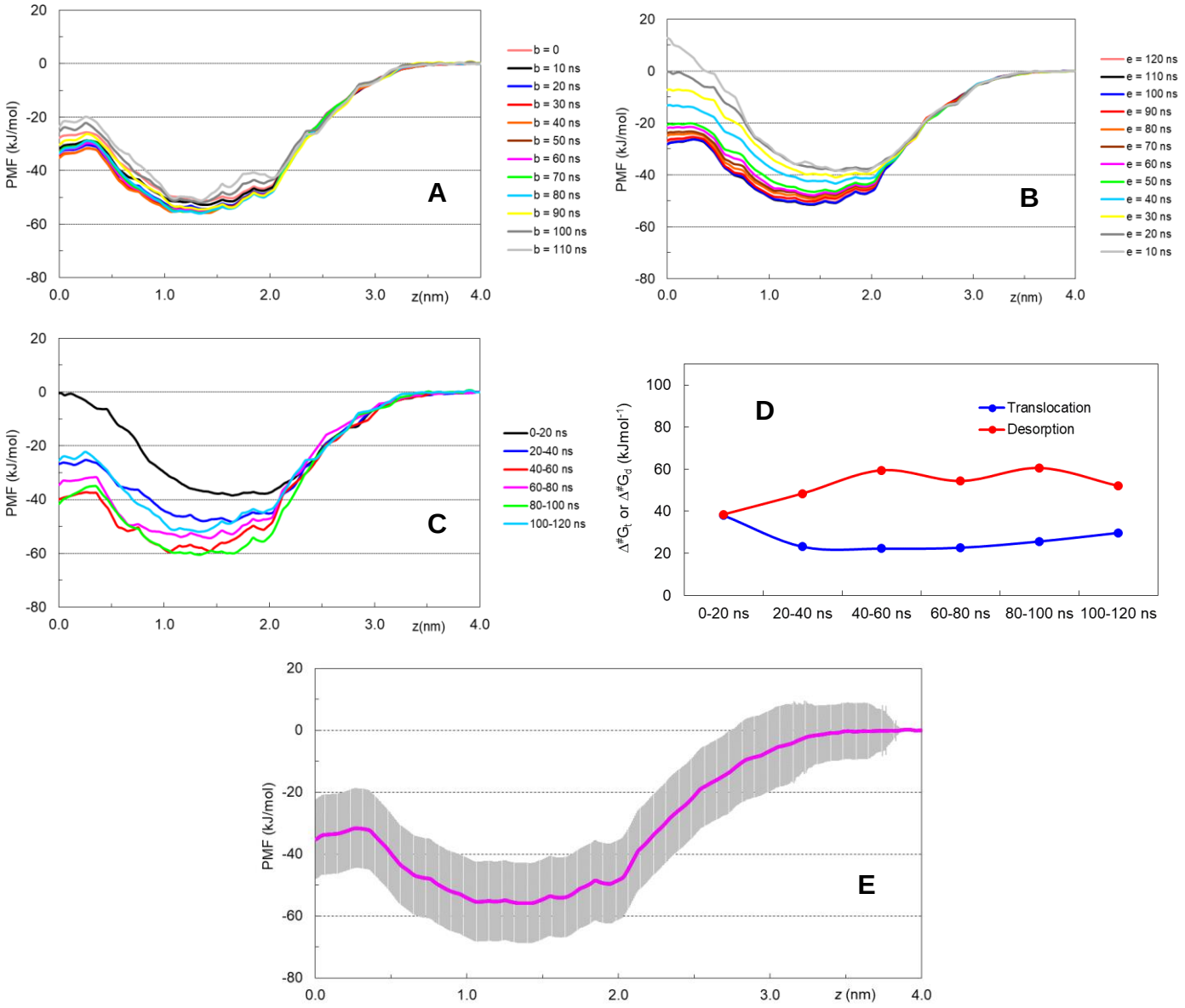

Figure S3. PMF error and convergence analysis for H(0). (A): Convergence of the PMF profiles obtained discarding initial simulation times. b = *t* denotes that times before *t* were not considered for analysis. (B): Convergence of the PMF profiles obtained discarding final simulation times. e = *t* denotes that times after *t* were not considered for analysis. (C): PMFs obtained considering different 20 ns time intervals of the sampling simulations. (D): Translocation and Desorption free energies ($\Delta^{\#}G_t$ and $\Delta^{\#}G_d$, respectively) calculated from each of the PMF curves of panel C. (E): PMF curve calculated using the last 80 ns of the 120 ns sampling runs.

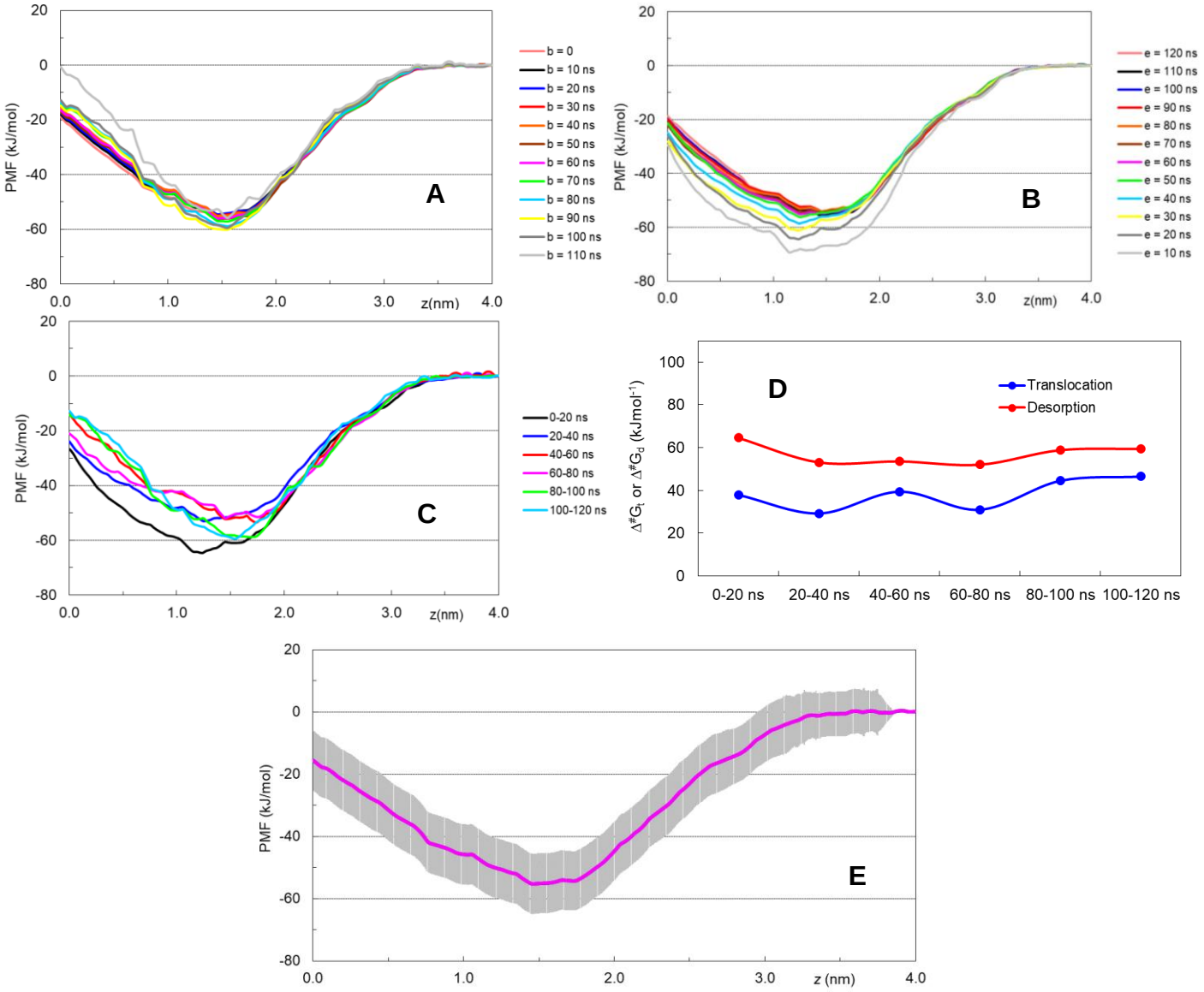

Figure S4. PMF error and convergence analysis for H(+1). Panels A-E have the same meanings as in Figure S3.

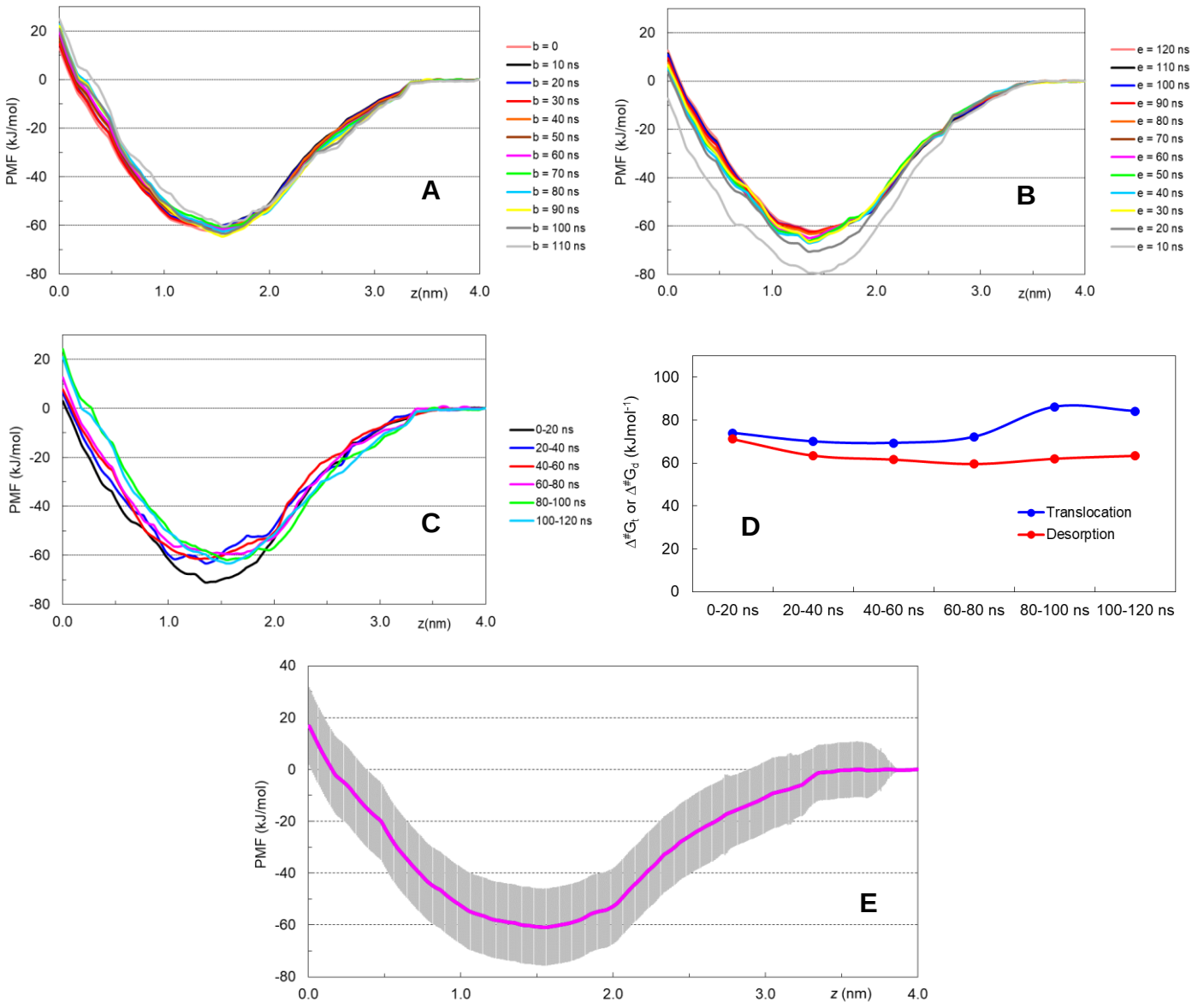

Figure S5. PMF error and convergence analysis for H(+2). Panels A-E have the same meanings as in Figure S3.