Iodide Binding in Sodium-Coupled Cotransporters

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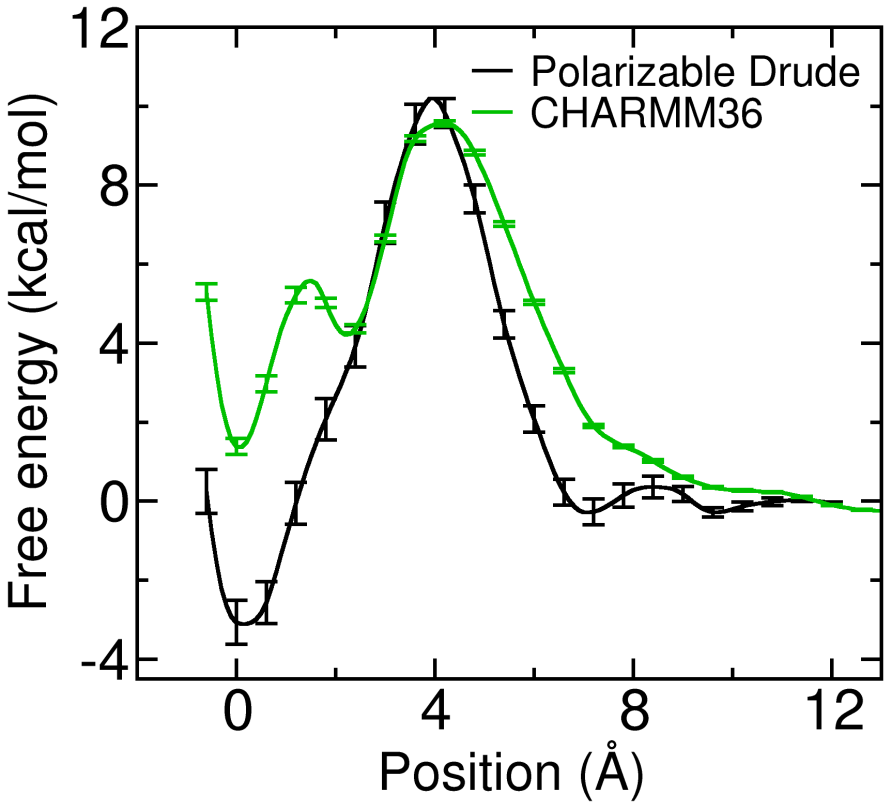

Figure S1: Importance of the using the Drude force field, which includes atomic polarizability, in the calculations described in the main text. The black curve shows the potential of mean force for iodide in a fragment of hNIS WT, presented in Fig. 6B of the main text. The green curve is the potential of mean force for an analogous system using the CHARMM36 force field, which does not represent atomic polarizability.

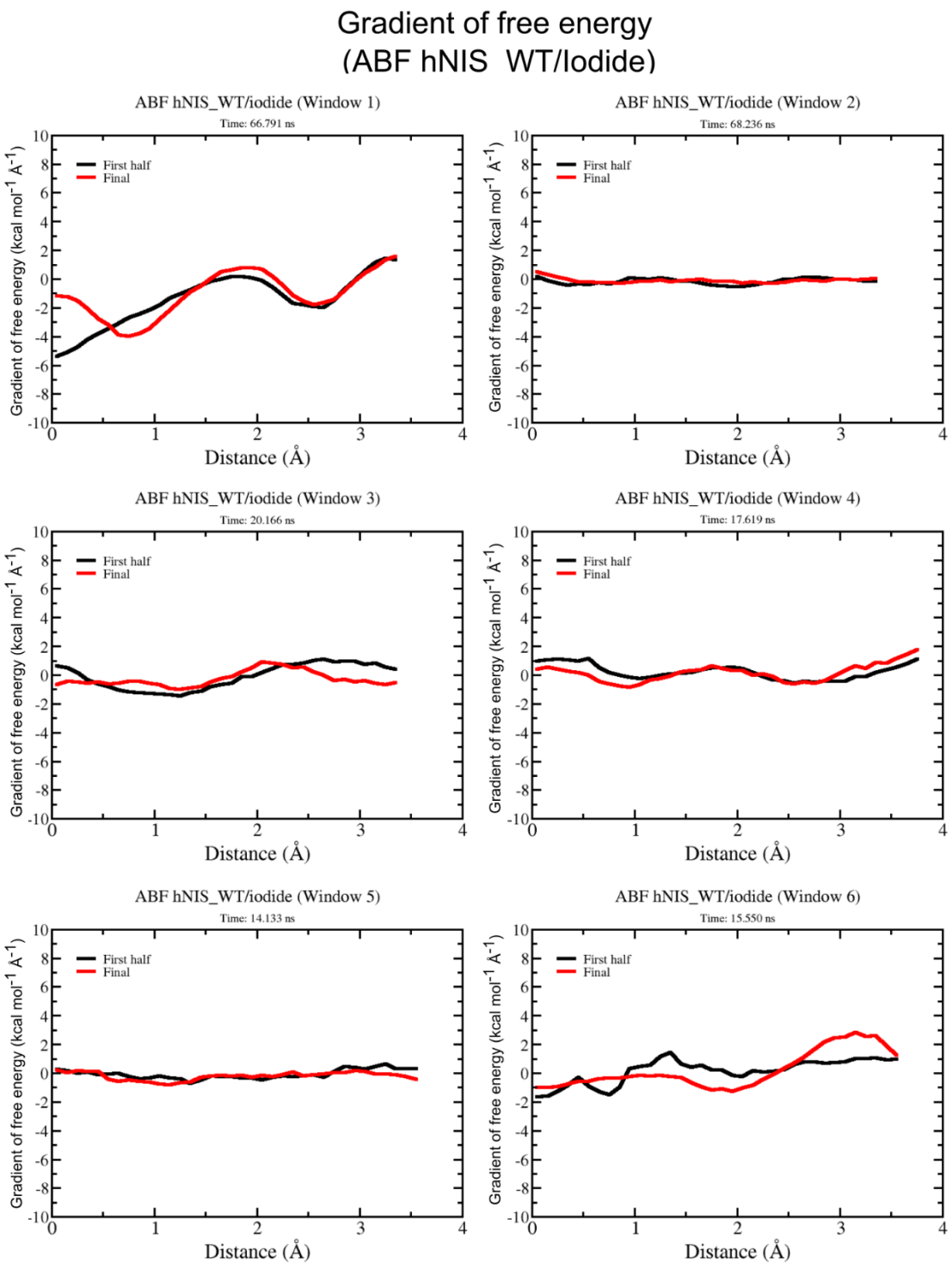

Figure S2: Convergence of the ABF calculations for wild-type hNIS interacting with iodide. The converged mean force was evaluated by comparing the gradient of the free energy of the first (black) and second (red) half of the length of the simulation for each of six segments defined along of the transition coordinate. The simulated total time is shown in each case.

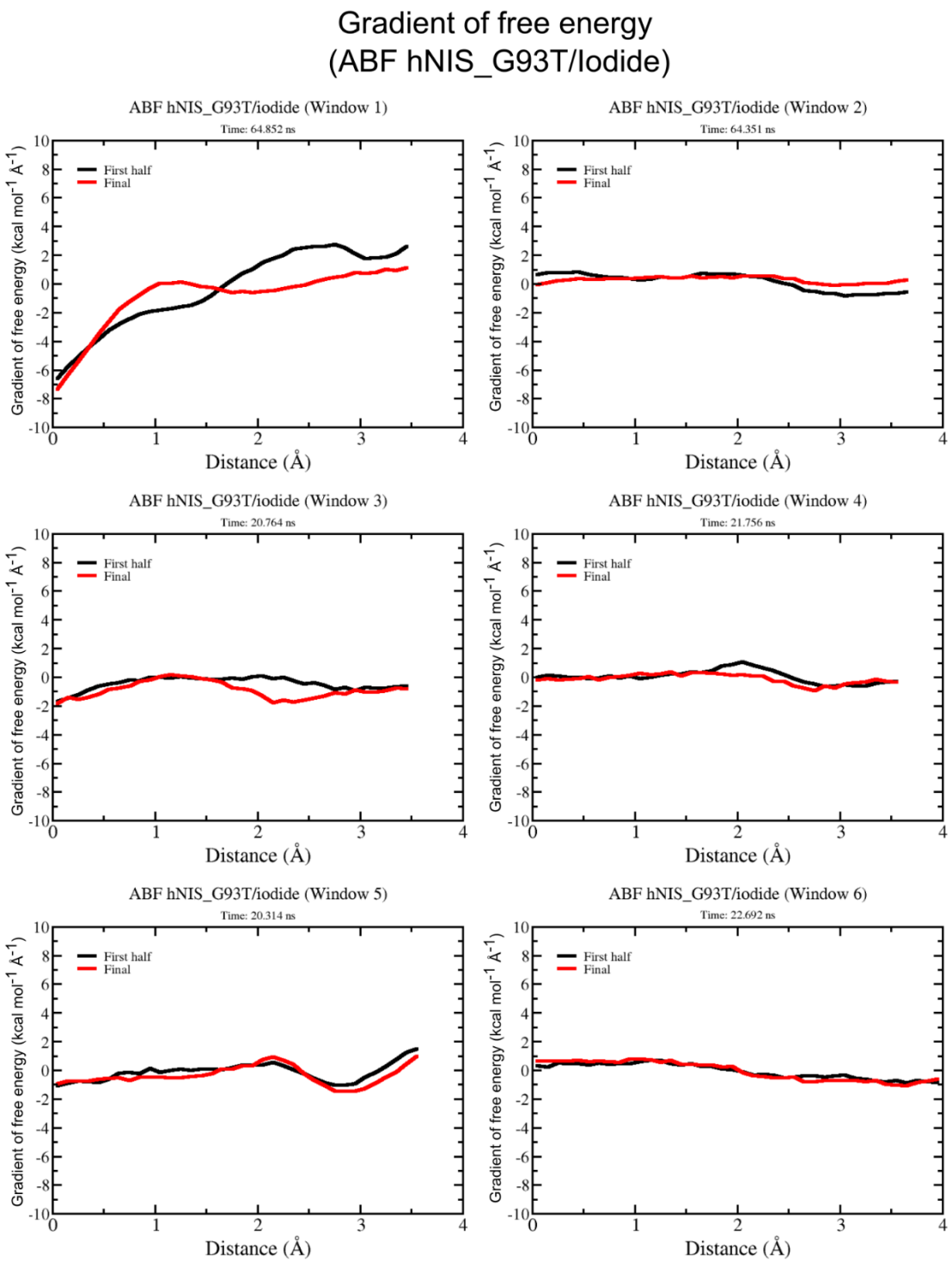

Figure S3: Convergence of the ABF calculations for G93T hNIS interacting with iodide. The converged mean force was evaluated by comparing the gradient of the free energy of the first (black) and second (red) half of the length of the simulation for each of six segments defined along of the transition coordinate. The simulated total time is shown in each case.

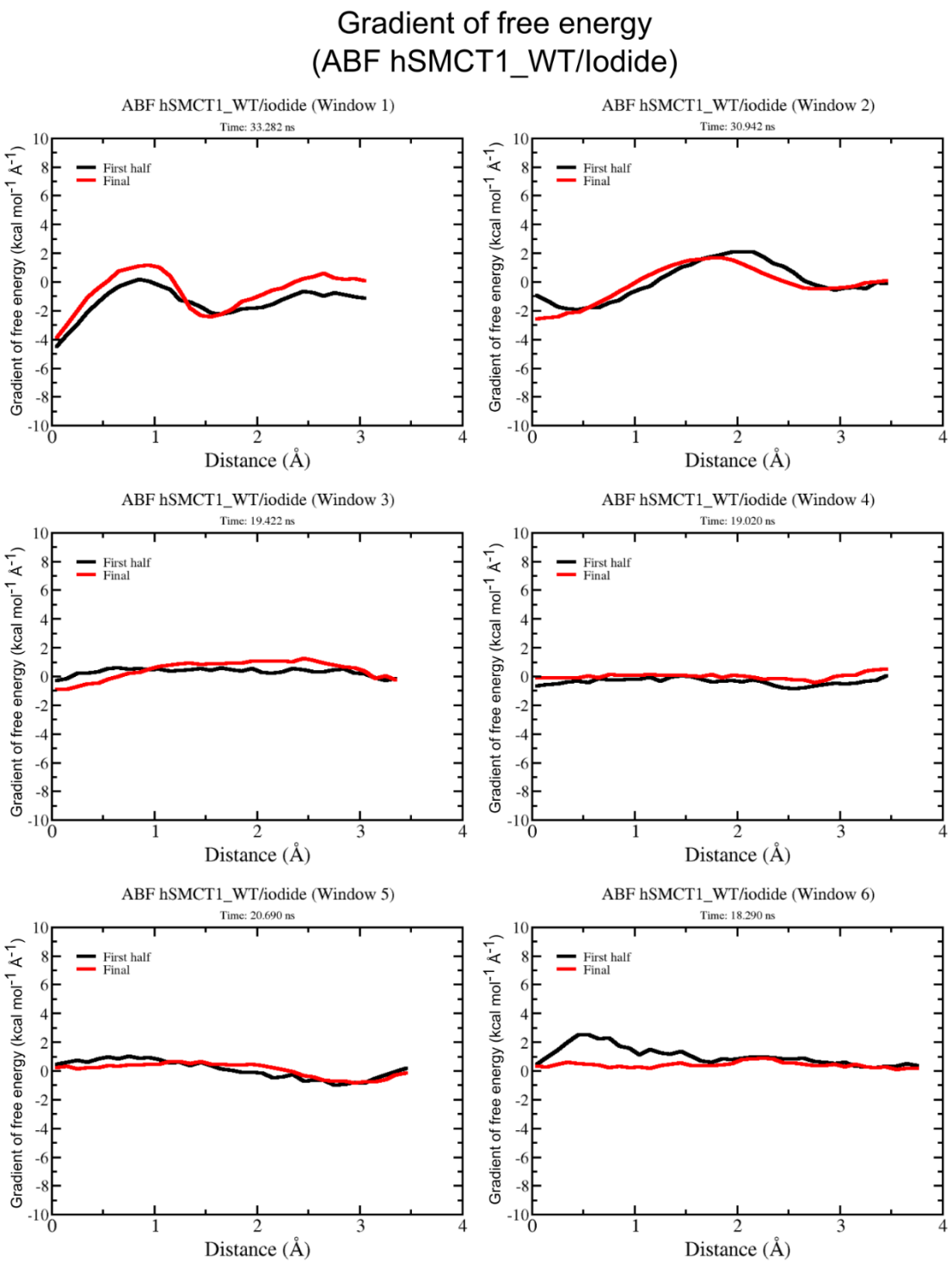

Figure S4: Convergence of the ABF calculations for wild-type hSMCT1 interacting with iodide. The converged mean force was evaluated by comparing the gradient of the free energy of the first (black) and second (red) half of the length of the simulation for each of six segments defined along of the transition coordinate. The simulated total time is shown in each case.

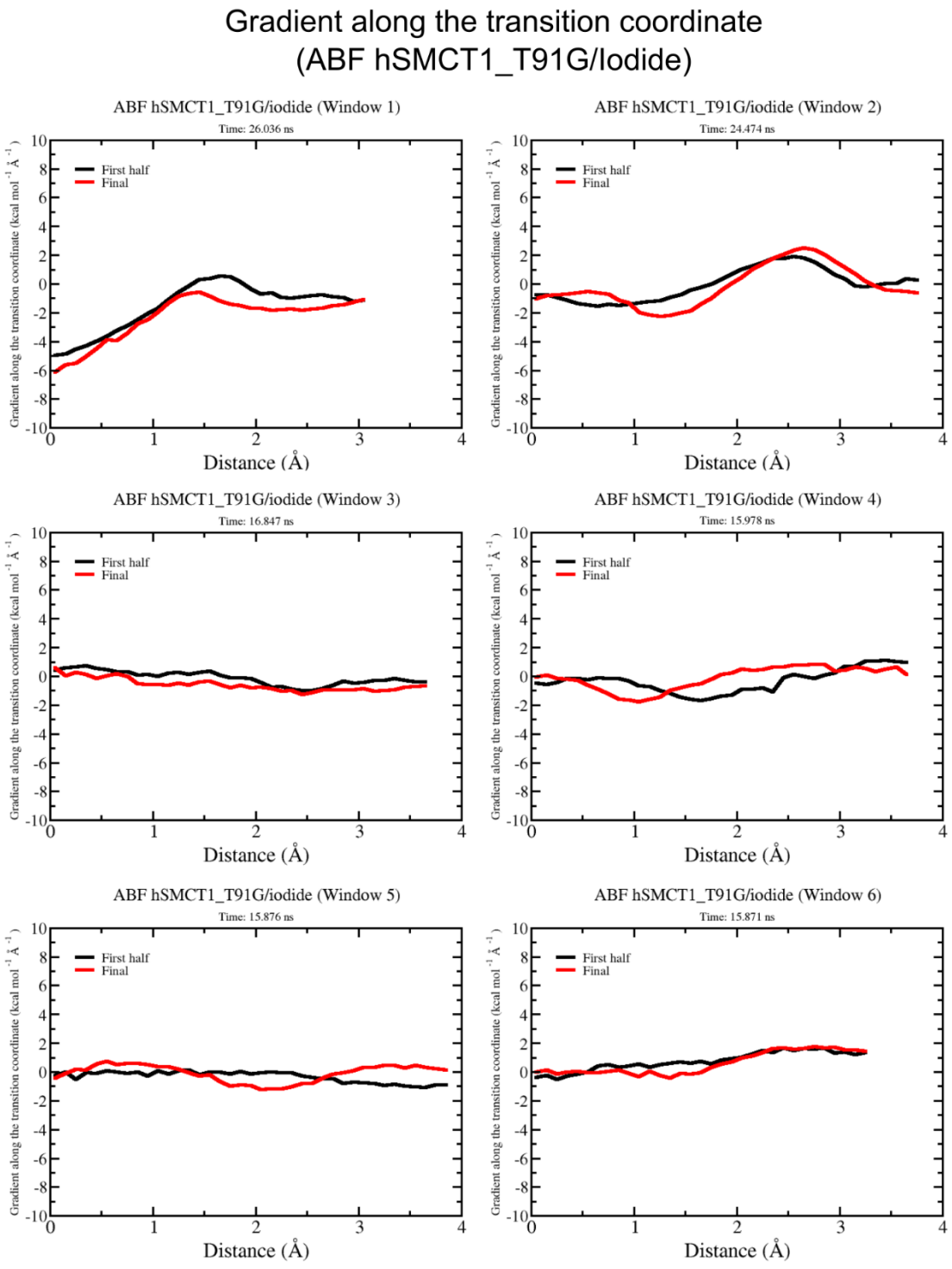

Figure S5: Convergence of the ABF calculations for T91G hSMCT1 interacting with iodide. The converged mean force was evaluated by comparing the gradient of the free energy of the first (black) and second (red) half of the length of the simulation for each of six segments defined along of the transition coordinate. The simulated total time is shown in each case.