Supplementary Information

Hybrid steered molecular dynamics approach to computing absolute binding free-energy for ligand-protein complexes---A brute force approach that is fast and accurate

Liao Y Chen

Department of Physics, University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249 USA

In Figs. S1 to S6, we provide details of the data produced in MD and SMD runs that are used to compute the binding affinities of binding caprylic acid to bovine lactoglobulin beta and binding glutathione to Schistosoma japonicum glutathione S-transferase tyrosine 7 to phenylalanine mutant.
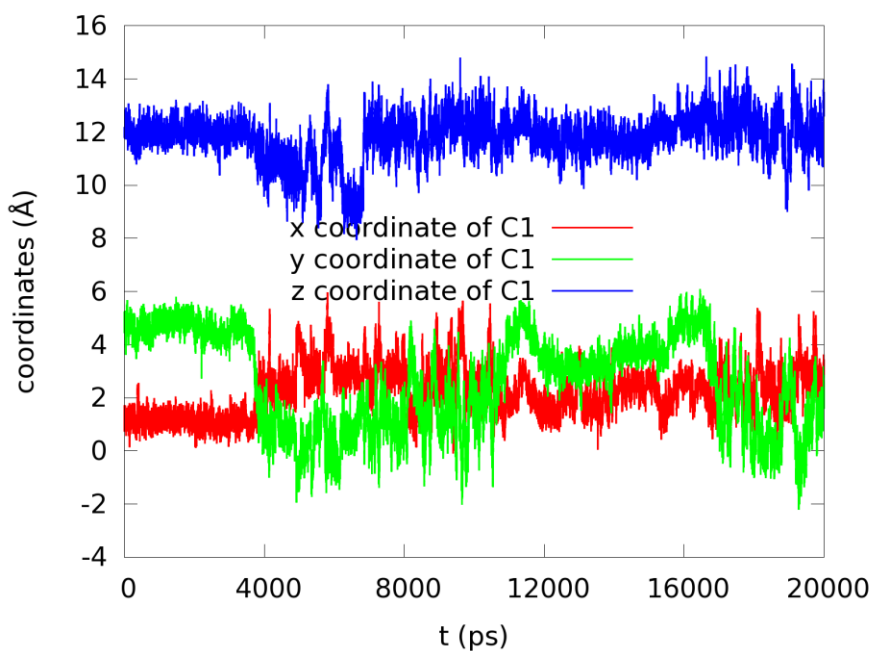

Fig. S1(a). Equilibrium fluctuations of C1's position in the bound state. These curves are for the last 20 ns of the total of 25 ns MD run.
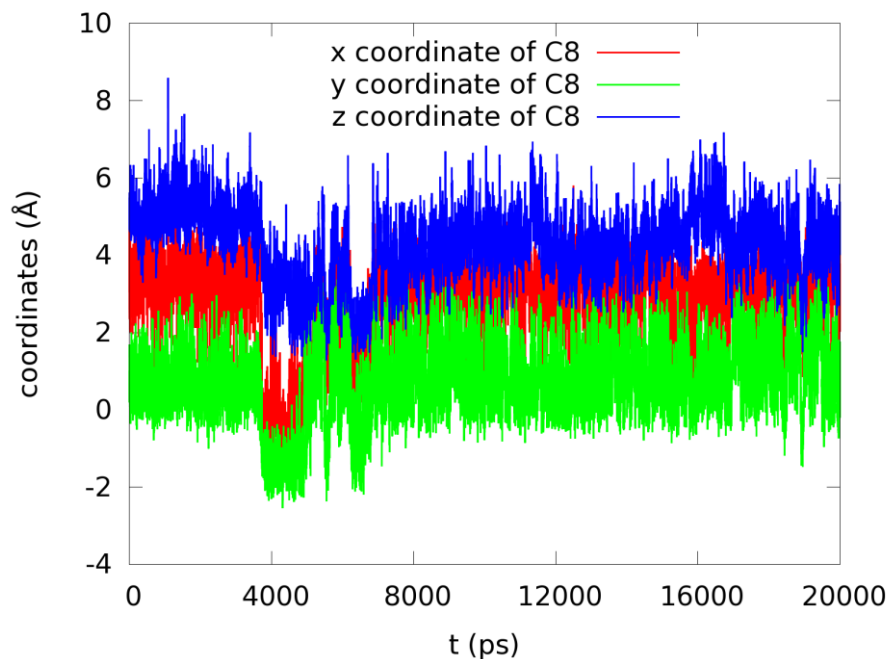
Fig. S1(b). Equilibrium fluctuations of C8's position in the bound state. These curves are for the last 20 ns of the total of 25 ns MD run.
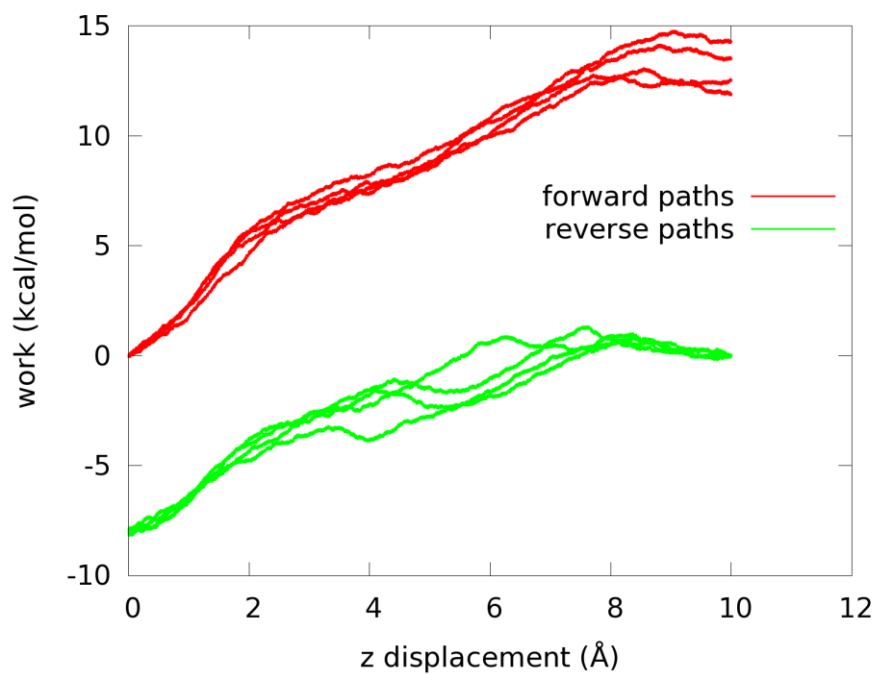

Fig. S2(a). Work done to the system along the pulling paths when C1 and C8 were pulled from the bound state to the dissociated state. These curves were used in BD-FDT to obtained the PMF curve shown in Fig. 3(a).
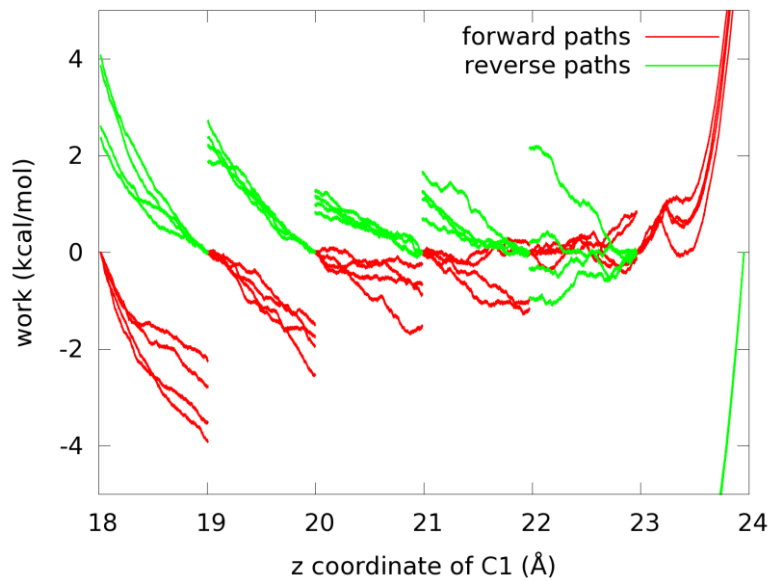
Fig. S2(b). Work done to the system along the pulling paths when C8 was fixed and C1 was pulled along the line connecting their positions in the dissociated states. These work curves were used in BD-FDT to obtain the PMF curve shown in Fig. 3(b).
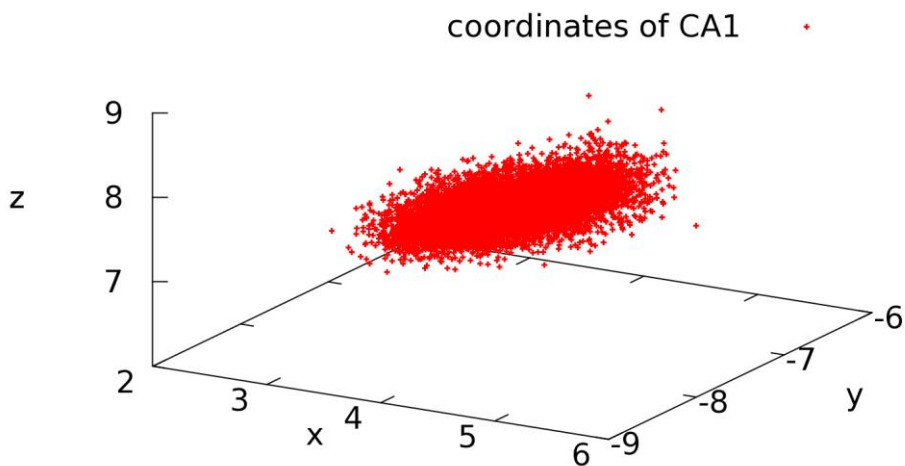

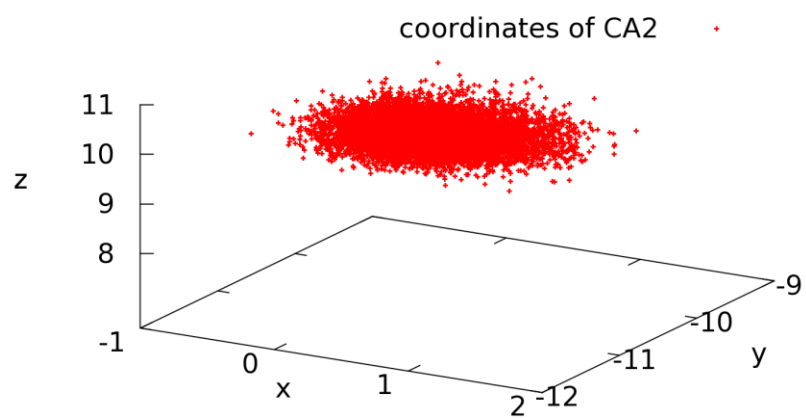Fig. S3(a). Equilibrium fluctuation of CA1 in the bound state.

coordinates of CA2

Fig. S3(b). Equilibrium fluctuation of CA2 in the bound state.
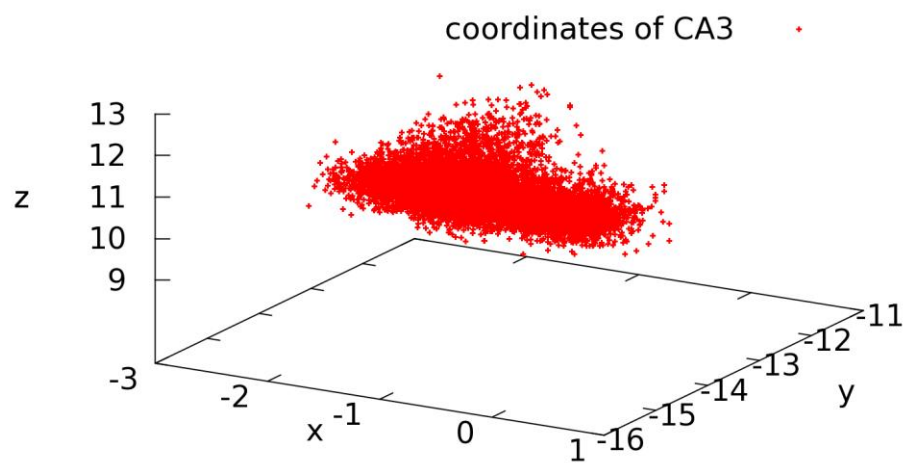
coordinates of CA3

Fig. S3(c). Equilibrium fluctuation of CA3 in the bound state.
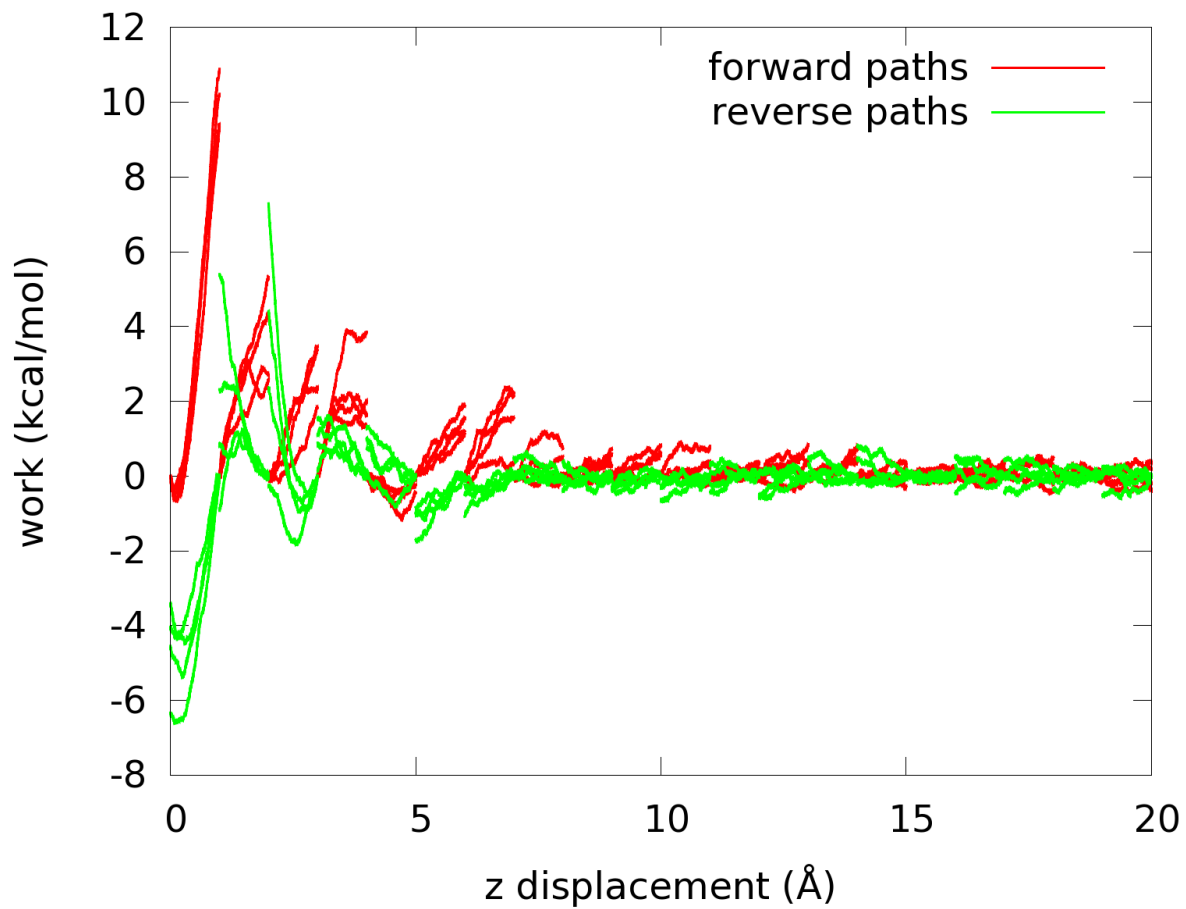
Fig. S4. Work done to the system along the pulling paths when CA1, CA2, and CA3 were pulled from the bound state to the dissociated state. These curves were used in BD-FDT to obtain the PMF curve shown in Fig. 5.
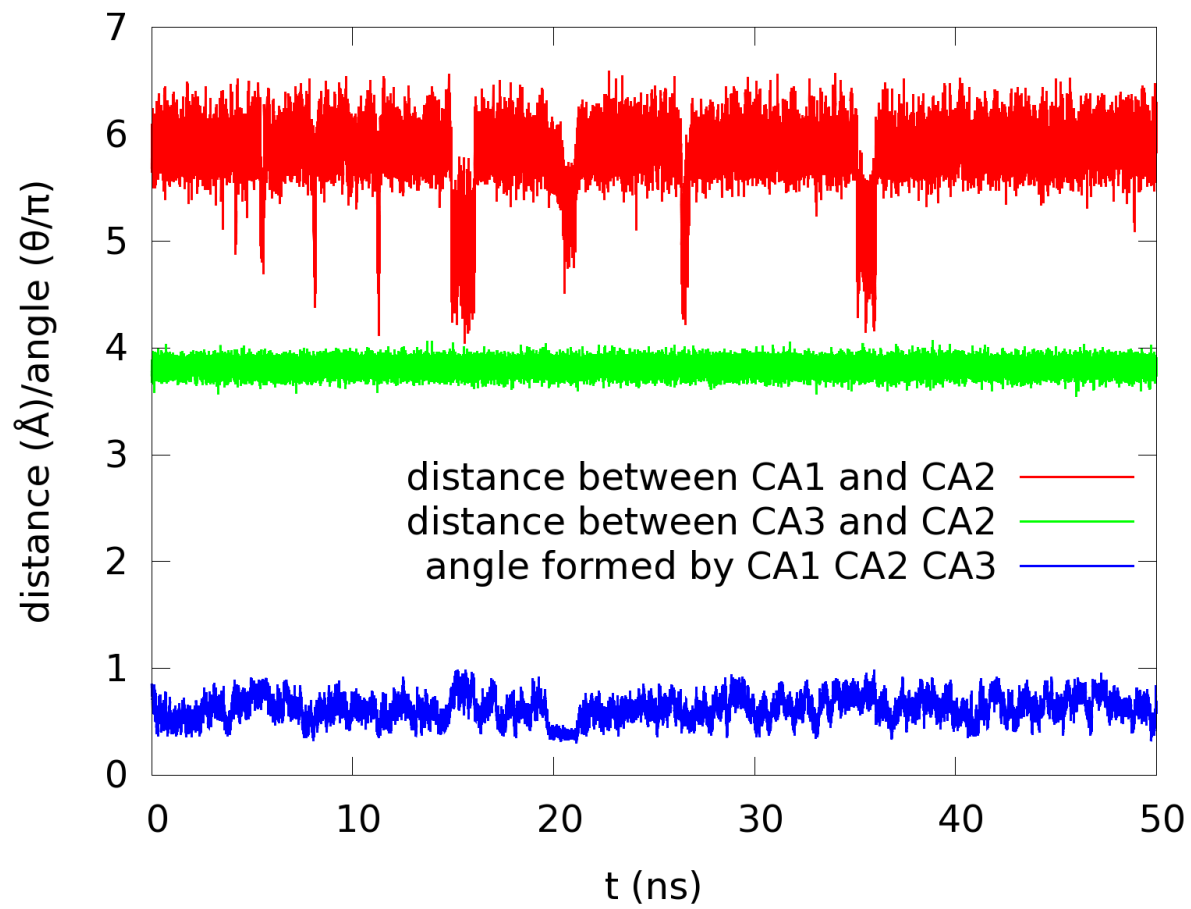
Fig. S5. Equilibrium fluctuation of CA1 and CA3 in the bulk when CA2 is fixed.
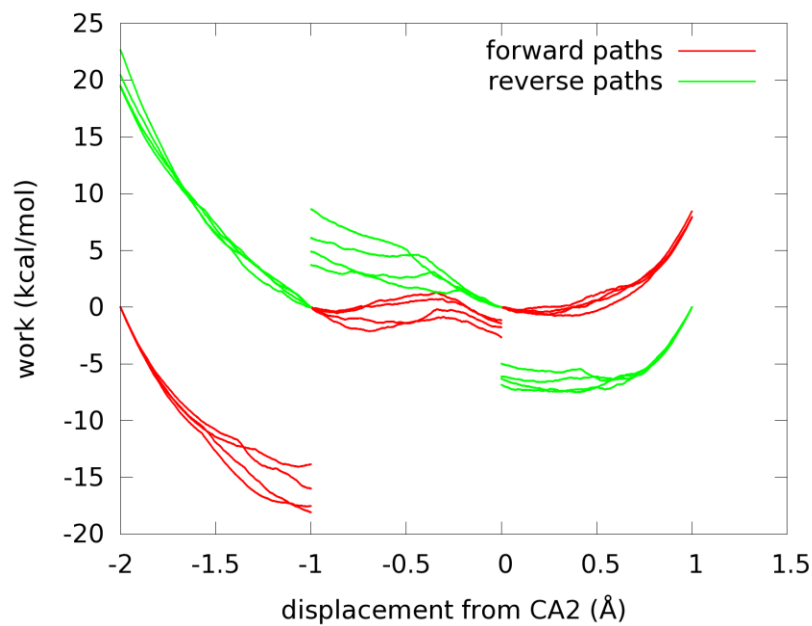
Fig. S6(a). Work done to the system along the pulling paths when CA2 was fixed and CA1 was pulled along the line connecting their positions in the dissociated states. These work curves were used in BD-FDT to obtain the PMF curve shown in Fig. 6(a).
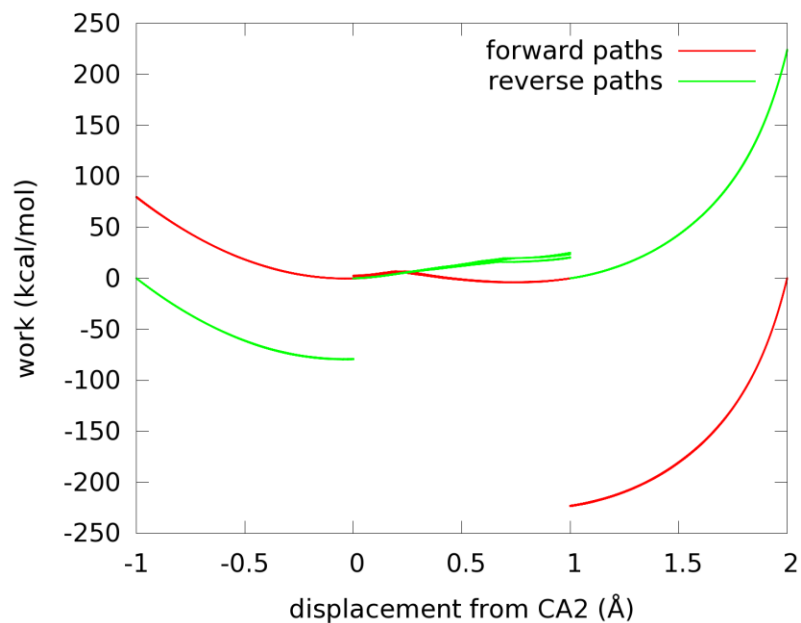

Fig. S6(b). Work done to the system along the pulling paths when CA2 was fixed and CA3 was pulled along the line connecting their positions in the dissociated states. These work curves were used in BD-FDT to obtain the PMF curve shown in Fig. 6(b).