Supplementary Data

Exploring Transition Pathway and Free Energy Profile of Large-scale Protein Conformational Change by Combining Normal Mode Analysis and Umbrella Sampling Molecular Dynamics

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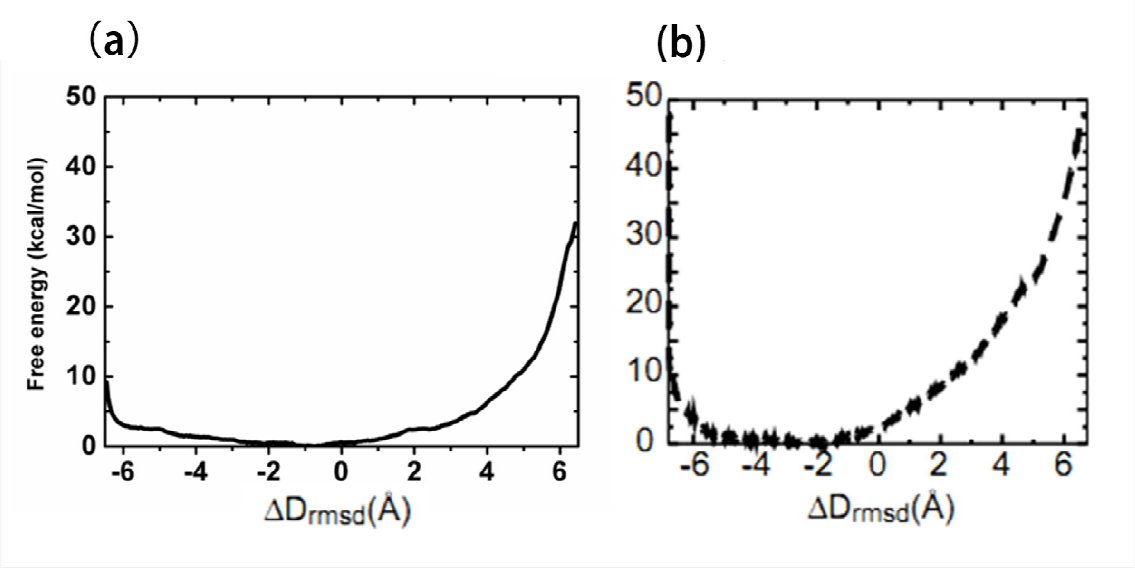

Figure S1. The one-dimensional free energy profiles as the function of ΔD_{rmsd} for the conformational transitions of apo AdK obtained (a) in the present study, and (b) in the previous molecular dynamics simulation study by Arora et al. Figures (b) is the Figure 2 (a) from the reference (Arora, K.; Brooks, C. L., *Proc Natl Acad Sci USA* **2007,** 104, 18496-18501). Reprinted with permission from Proc Natl Acad Sci USA.

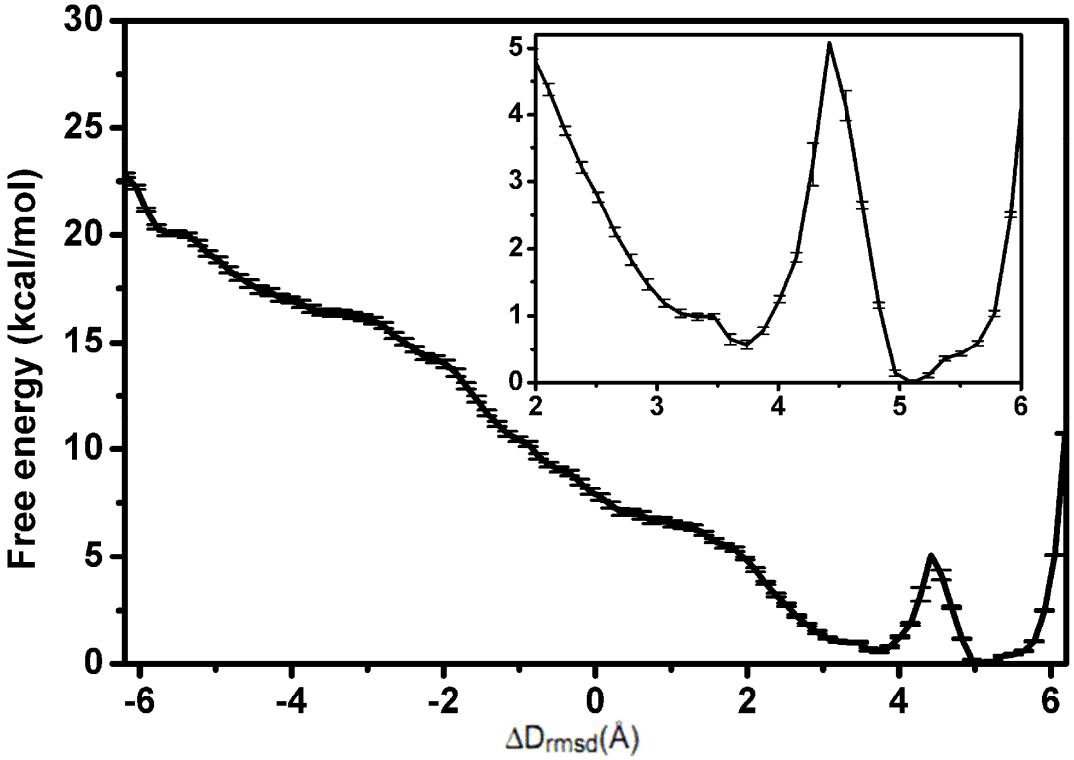

Figure S2. The one-dimensional free energy profile as the function of ΔD_{rmsd} and the corresponding error bar for the conformational transition of ligand-bound AdK.