Supplementary Data

Mapping Central α-Helix Linker Mediated Conformational Transition Pathway of Calmodulin via Simple Computational Approach

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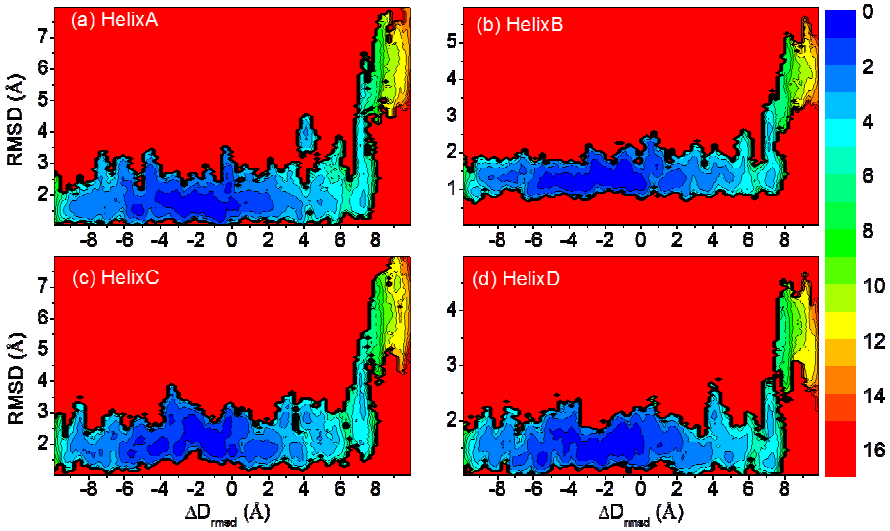

Figure S1. Two-dimensional free energy profiles as the function of ΔD_{rmsd} of intact apo-CaM and the RMSD value of individual helices within N-terminal domain to their respective closed states. The contours are spaced at intervals of 1.0 kcal/mol.

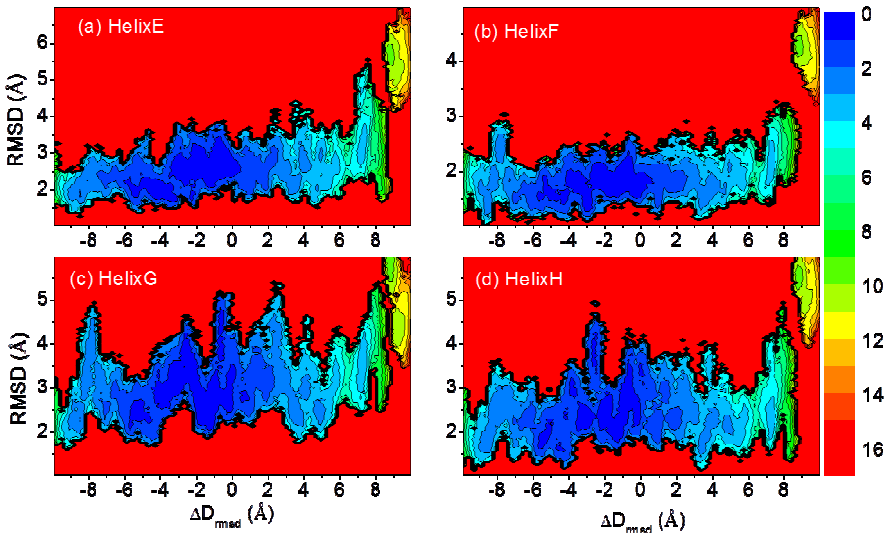

Figure S2. Two-dimensional free energy profiles as the function of ΔD_{rmsd} of intact apo-CaM and the RMSD value of individual helices within C-terminal domain to their respective closed states. The contours are spaced at intervals of 1.0 kcal/mol.

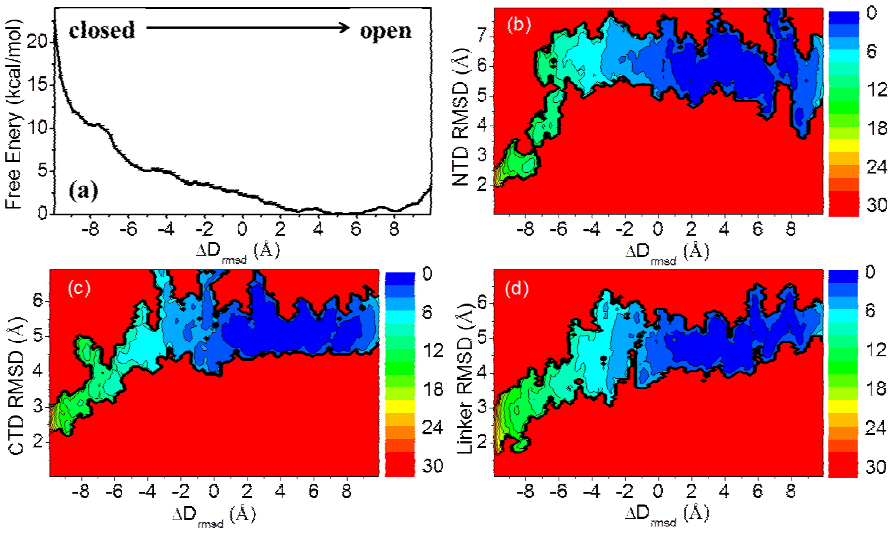

Figure S3. (a) One-dimensional free energy profiles as a function of ΔD_{rmsd} for the conformational transition of Ca^{2+}-bound calmodulin. (b-d) Two-dimensional free energy landscapes for the conformational transition of Ca^{2+}-bound calmodulin as the function of ΔD_{rmsd} and the RMSD value of different regions (N-terminal domain, C-terminal domain, central α-helix linker) to their closed states. The contours are spaced at intervals of 2.0 kcal/mol.

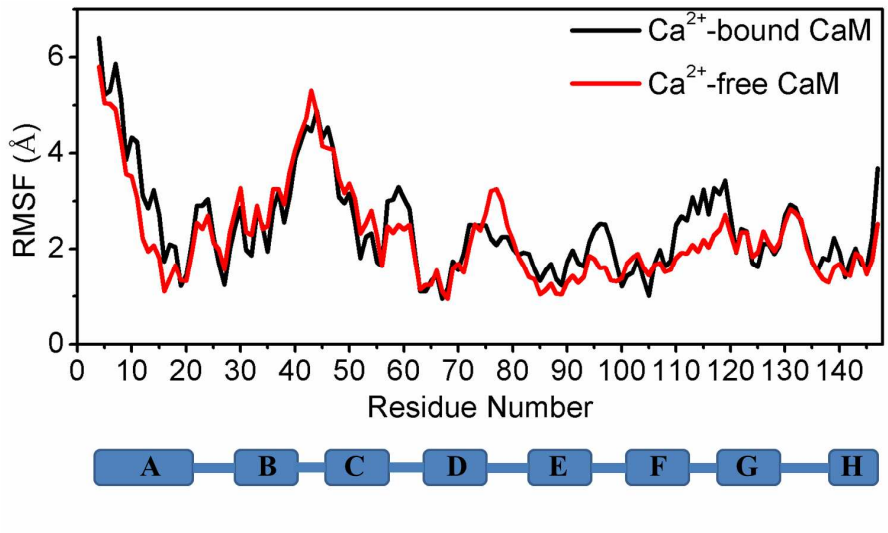

Figure S4. The room-mean-square-fluctuation (RMSF) *vs* sequence index in Ca^{2+}-free and Ca^{2+}-bound calmodulin measured from conventional MD simulation. The helix secondary structure is indicated below the plot.