Supporting Information for

Efficient Conformational Search Based on Structural Dissimilarity Sampling: Applications for Reproducing Structural Transitions of Proteins

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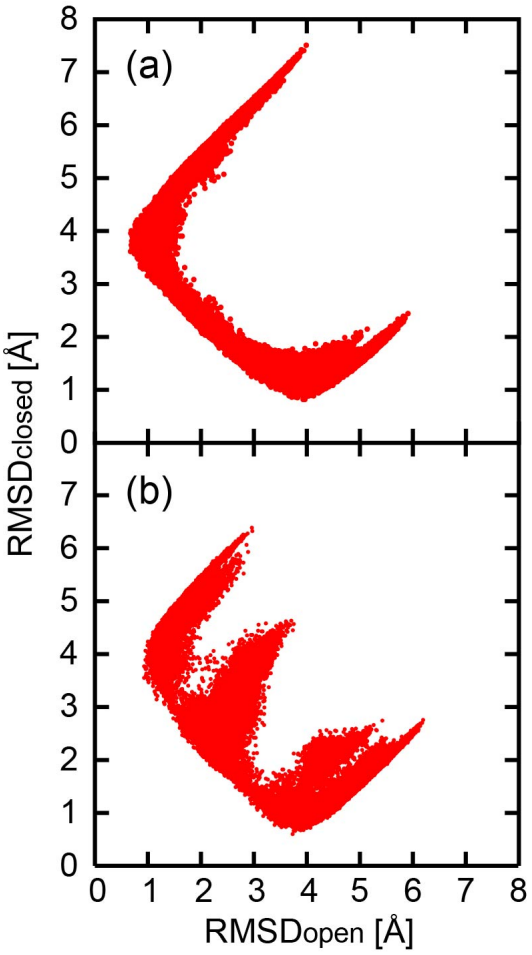
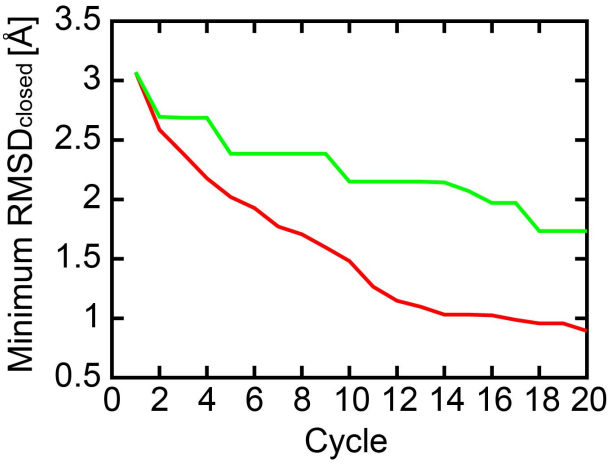
Supporting Information (Figure S1)



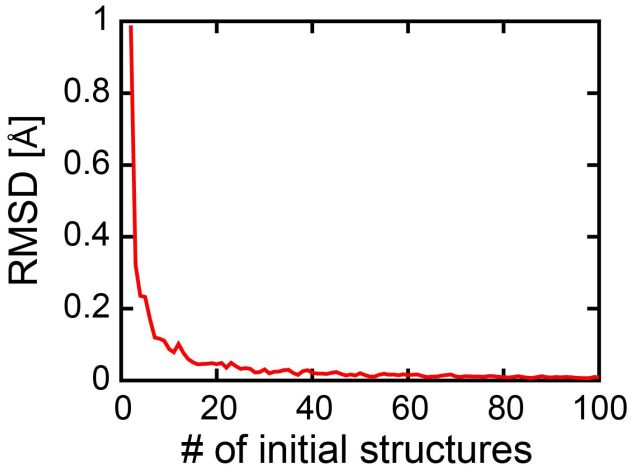
Projections of all the trajectories generated by the trials of SDS ($N_{initial}$ = 100 and DOF = 30 PCs), starting from (a) the open and (b) closed states of MBP during the 50 cycles. Each snapshot was projected onto the two-dimensional conformational subspace spanned by C_α RMSD measured from the open and closed forms, ($RMSD_{open}$, $RMSD_{closed}$).

Supporting Information (Figure S2)



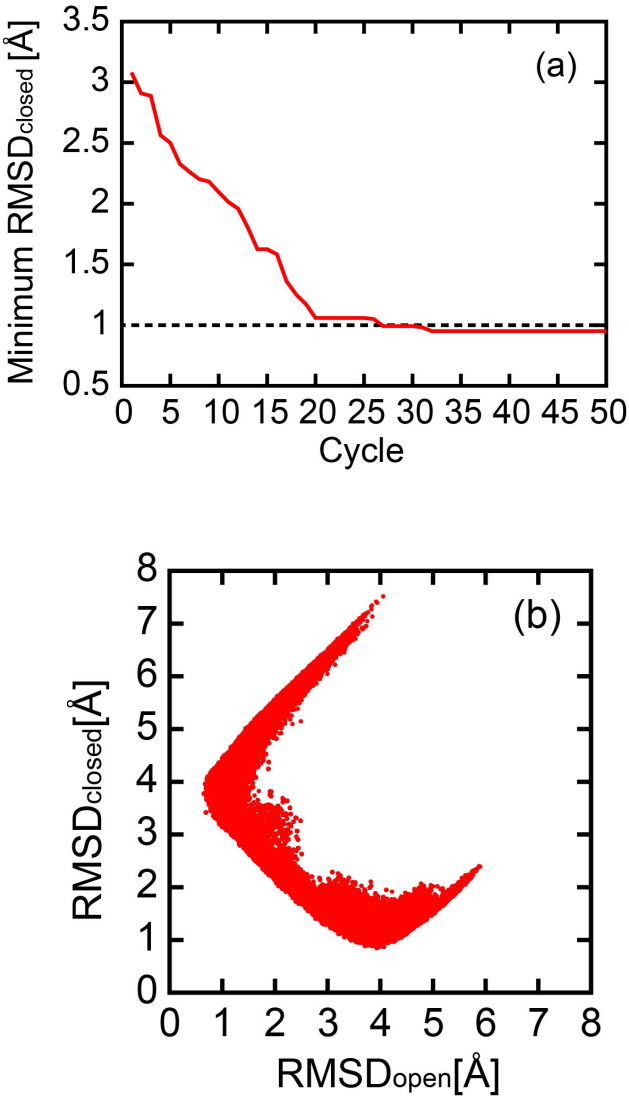
(red) Profile of the minimum C_α RMSD measured from the closed form of MBP, $RMSD_{closed}$, for the trial ($N_{initial}$ = 100 and DOF = 30 PCs). (green) Profile of the minimum $RMSD_{closed}$ for the trial ($N_{initial}$ = 100) using the inner products defined by the atomic configuration (C_α coordinates).

Supporting Information (Figure S3)



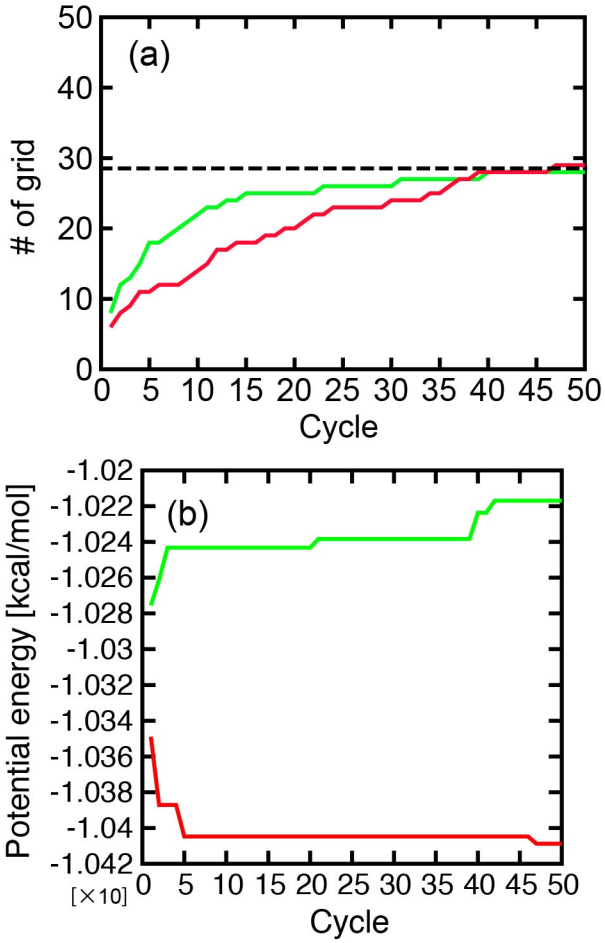
Profile of C_α RMSD among average structures constructed by a different set of initial structures selected at the 1st cycle for the trial of SDS starting from the open form of MBP ($N_{initial}$ = 100 and DOF = 30 PCs).

Supporting Information (Figure S4)



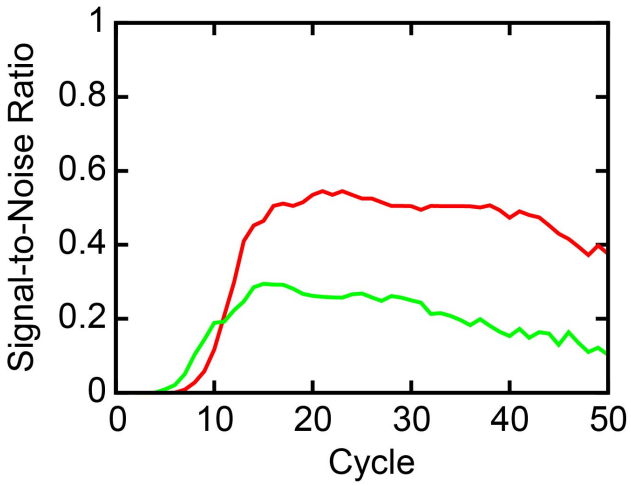
(a) Profile of the minimum C_α RMSD measured from the closed form of MBP ($RMSD_{closed}$) for the trial of SDS ($N_{initial}$ = 50 and DOF = 30 PCs). (b) Projections of all the trajectories of the trial during the 50 cycles.

Supporting Information (Figure S5)



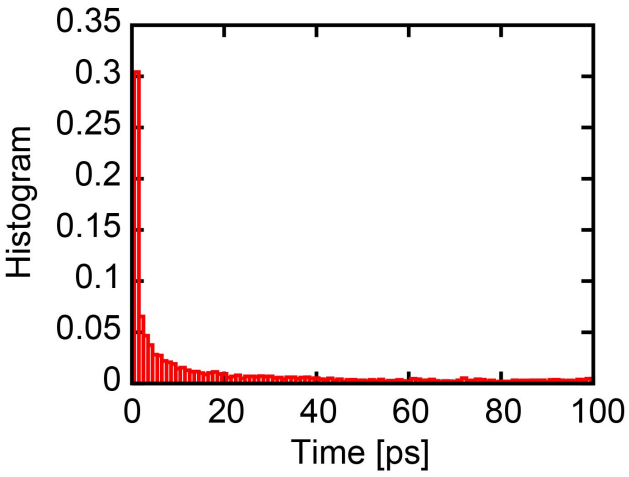
(a) Profile of convergence of conformational resampling by SDS. The grids were defined as finite cells in one-dimensional conformational subspace spanned by $RMSD_{closed}$, and total numbers of the grids were monitored. Profiles for the trial of SDS starting from the (red) open and (green) closed of forms of MBP ($N_{initial}$ = 100 and DOF = 30 PCs). The dashed line represents convergence of conformational resampling. (b) Profiles of the (red) minimum and (green) maximum potential energies for the trial of SDS starting from the open form of MBP ($N_{initial}$ = 100 and DOF = 30 PCs).

Supporting Information (Figure S6)



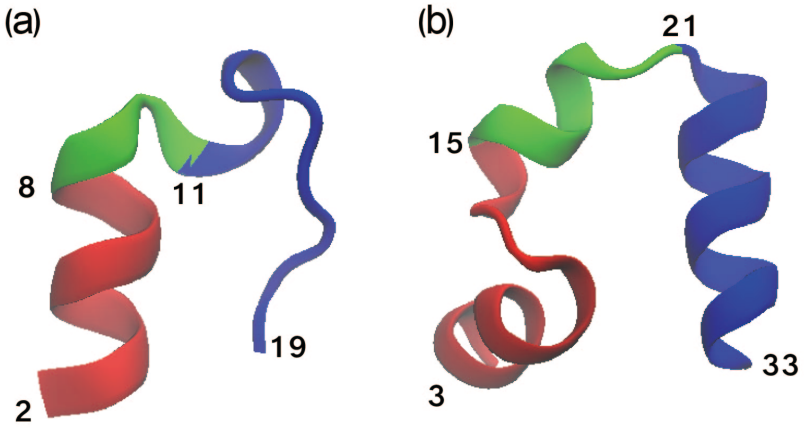
Signal-to-Noise ratio of the trials of SDS starting from the (red) open and (green) closed forms of MBP ($N_{initial}$ = 100 and DOF = 30 PCs).

Supporting Information (Figure S7)



Histogram of snapshots for time at which they were selected as initial structures from the 100-ps MD simulations during the cycles of conformational resampling for the trial of SDS starting from the open form of MBP (N_{initial} = 100 and DOFs = 30 PCs) during the 50 cycles.

Supporting Information (Figure S8)



Experimentally determined structures of (a) trp-cage and (b) villin at their native states. Segment1 (red and green regions) consisting of the residues (2-11) for trp-cage and (3-21) for villin, Segment2 (green and blue regions) consisting of the residues (8-19) for trp-cage and (15-33) for villin. The common region between segments1 and segment2 are colored in green.