Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Unveiling Conformational Dynamics Changes of H-Ras Induced by Mutations Based on Accelerated Molecular Dynamics

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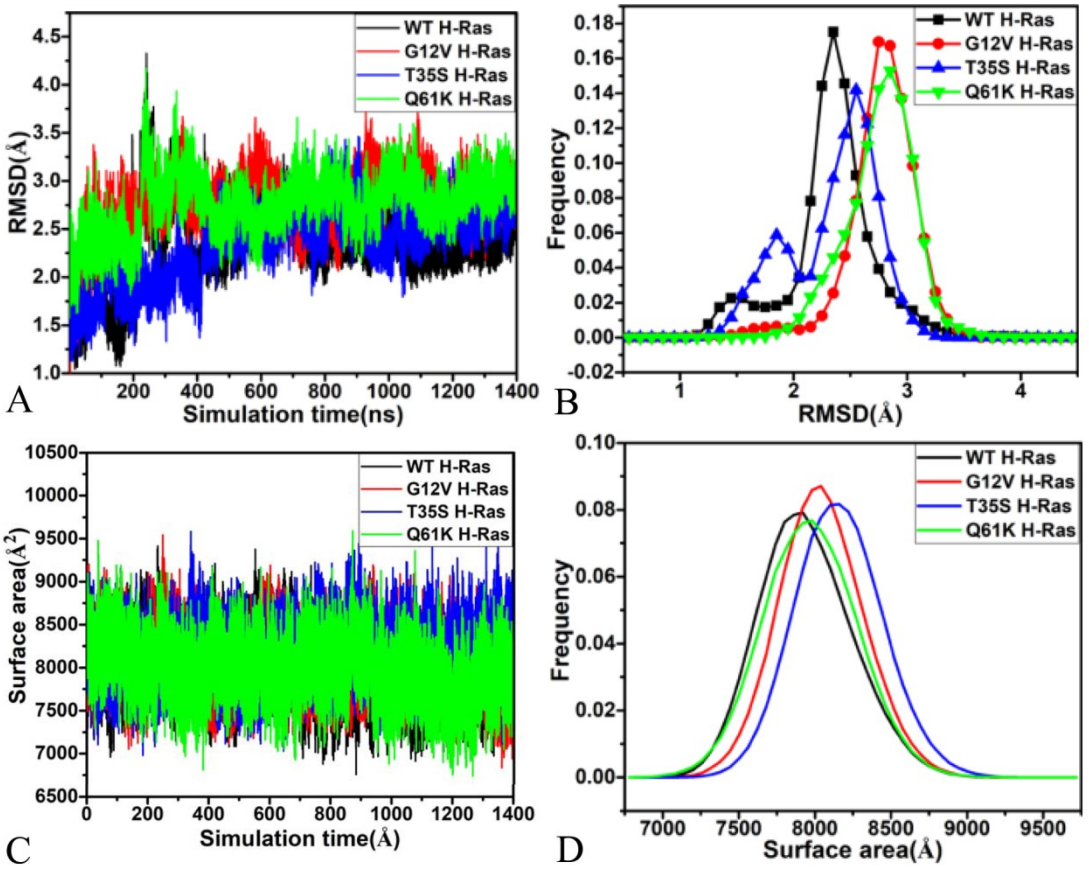

Fig. S1 Root-mean-square deviations (RMSDs) and surface area: (A) the evolutions of RMSDs of backbone atoms in the WT and mutated H-Ras as the simulation time, (B) frequency distributions of RMSDs, (C) the function of molecular surface area over the simulation time and (D) frequency distributions of molecular surface area.

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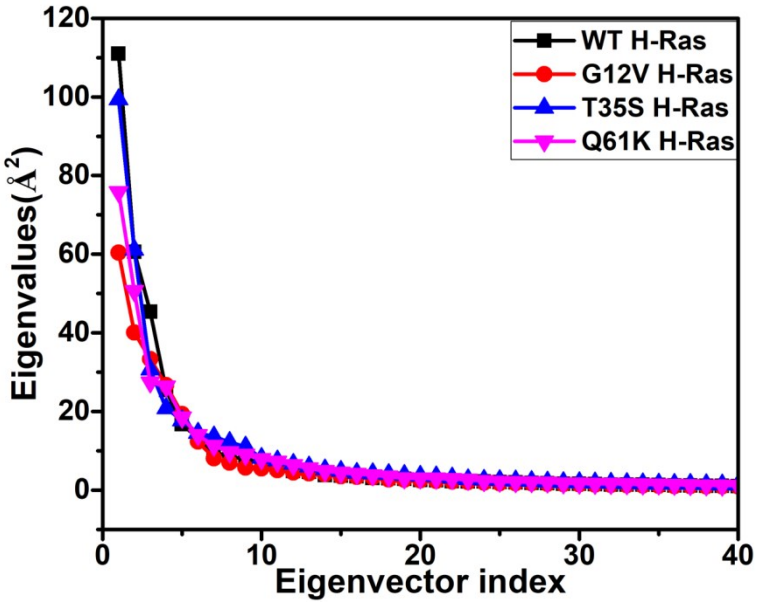

Fig. S2 Eigenvalues reflecting total motion strength of the GNP-bound WT and mutated H-Ras versus the corresponding eigenvector indices.

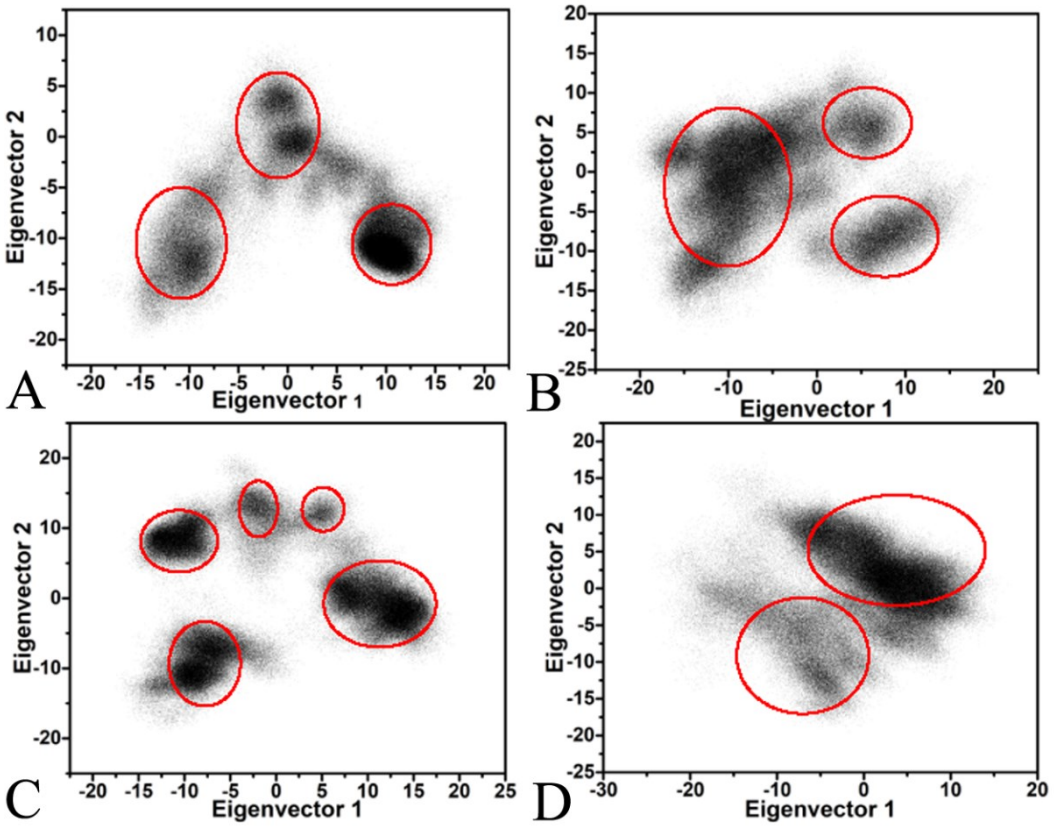

Fig. S3 Projections of aMD trajectories on the first two eigenvectors from PC analysis: (A) the WT H-Ras, (B) the G12V mutated H-Ras, (C) the T35S mutated H-Ras and (D) the Q61K mutated H-Ras.

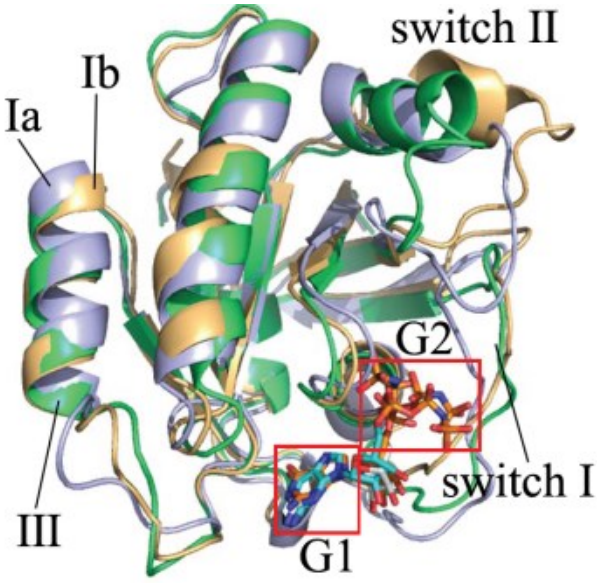

Fig. S4 Superimposition of the structures Ⅰa, Ⅰb and Ⅲ of the GNP-bound WT H-Ras sampled by the aMD simulation, in which H-Ras is shown in cartoon modes and GNP is displayed in stick style. G1 represents the guanylate ester group of GNP and G2 indicates the phosphoaminophosphonic acid group of GNP.

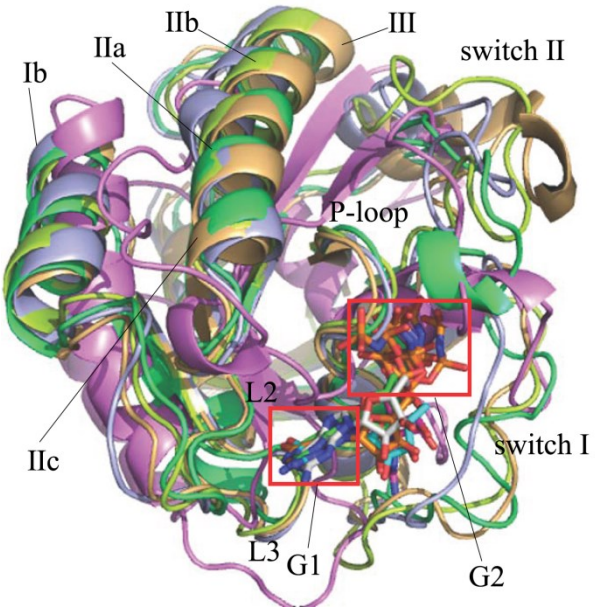

Fig. S5 Superimposition of the structures Ⅰb, Ⅱa, Ⅱb, Ⅱc and Ⅲ of the GNP-binding T35S H-Ras sampled by the aMD simulation, in which H-Ras is shown in cartoon modes and GNP is displayed in stick modes. G1 represents the guanylate ester group of GNP and G2 indicates the phosphoaminophosphonic acid group of GNP.

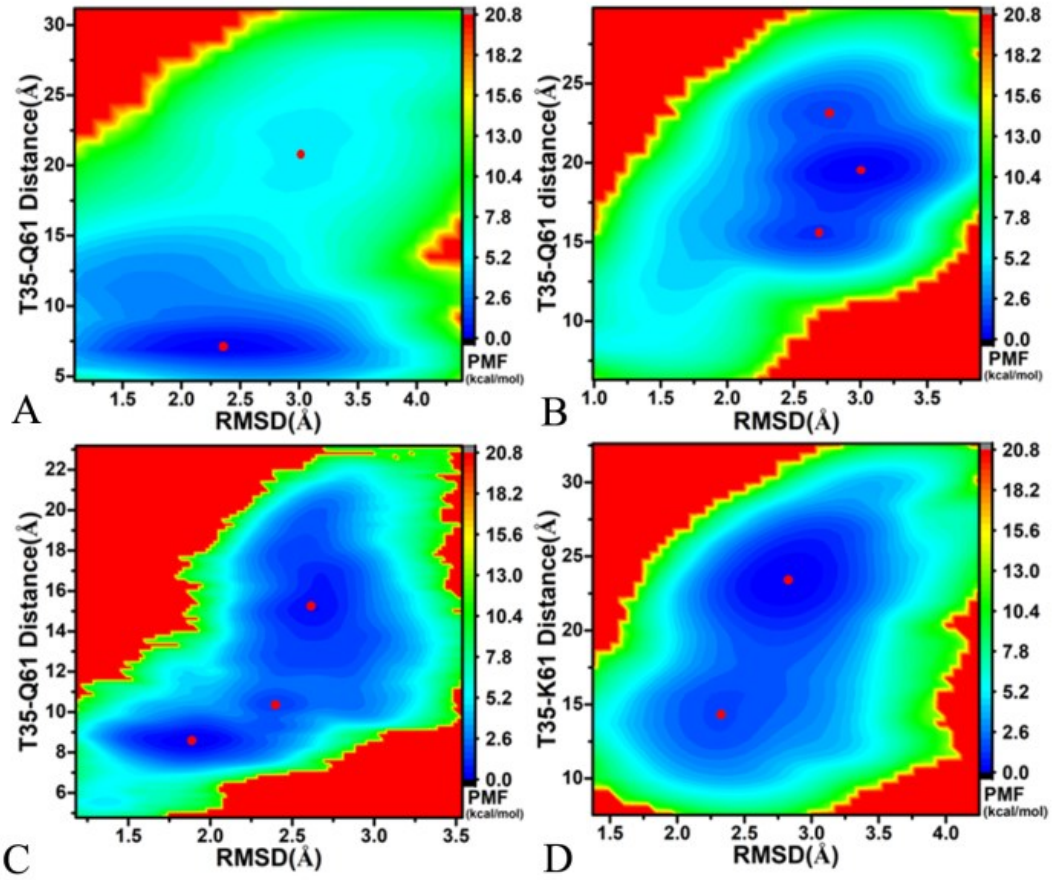

Fig. S6 Free energy landscapes built by utilizing RMSDs of backbone and the distance between T35 and the residue 61 as reaction coordinates: (A) the GNP-bound WT H-Ras, (B) the GNP-bound G12V H-Ras, (C) the GNP-bound T35S H-Ras and (D) the GNP-bound Q61K H-Ras.