Supporting Material

Computational study of Tat-CDK9-Cyclin binding dynamics and its implication in transcription-dependent HIV latency

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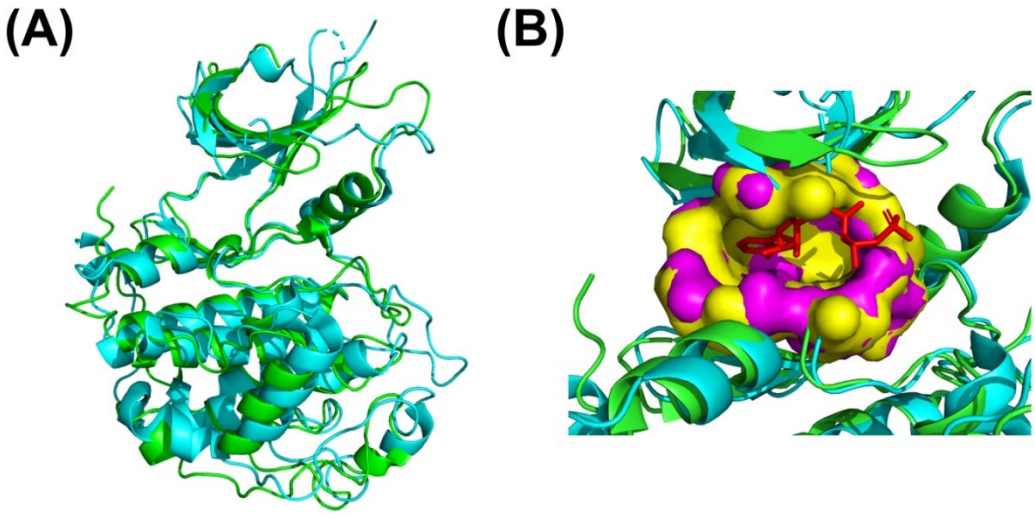

Fig. S1. The structural homology analysis of CDK2 and CDK9. (A) The RMSD between CDK2 (PDB ID: 1FIN, colored in cyan) and CDK9 (PDB ID: 5L1Z, colored in green) structures is 1.23 Å. (B) The volume values of the ATP-binding pocket of CDK2 (colored in magenta) and CDK9 (colored in yellow) are 482.18 $Å^3$ and 502.59 $Å^3$. These two ATP-binding pockets are very similar with an RMSD of 0.58 Å. The ATP pockets were identified using DoGSiteScorer.

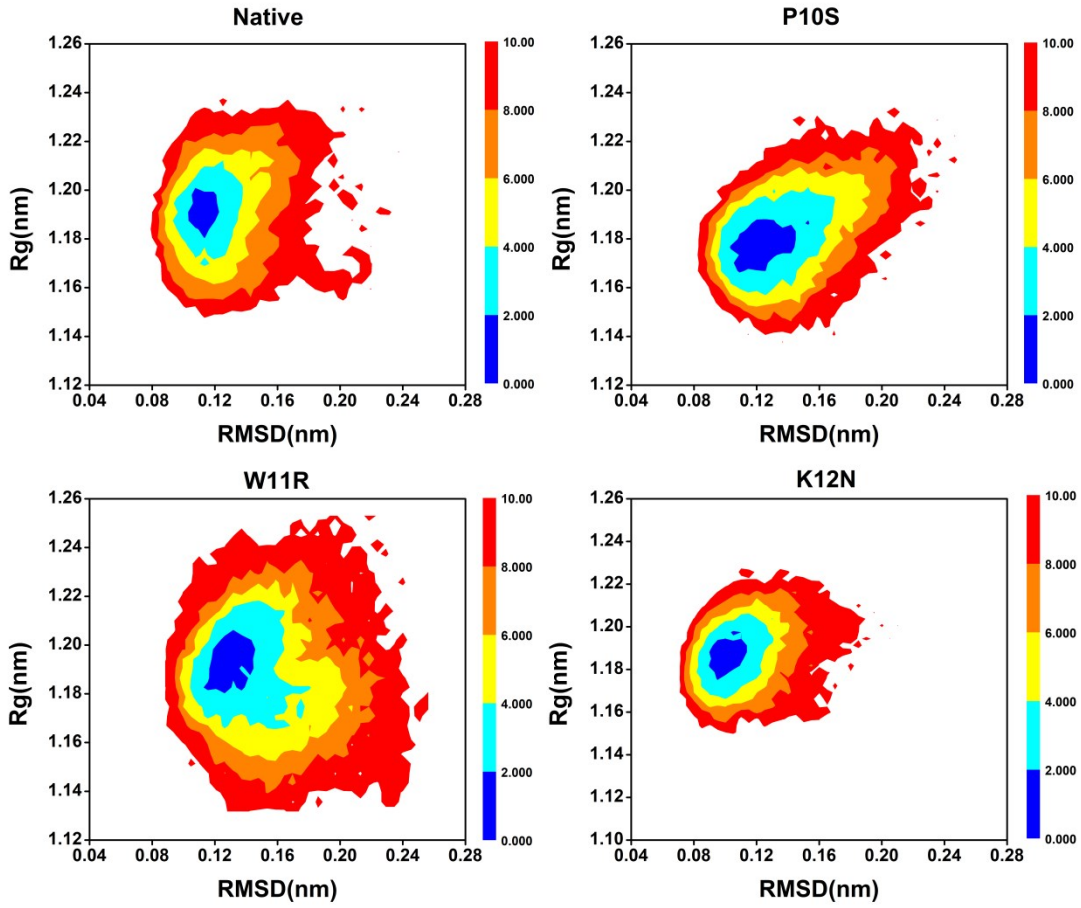

Fig. S2. Two-dimensional free energy landscapes from the last 30ns simulations. The X-axis and Y-axis are RMSD and radius of gyration. The color is scaled according to kcal/mol. Blue color indicates a lower energy structure in the MD trajectory. The results suggest that all of the molecular dynamics simulations fell into stable states.

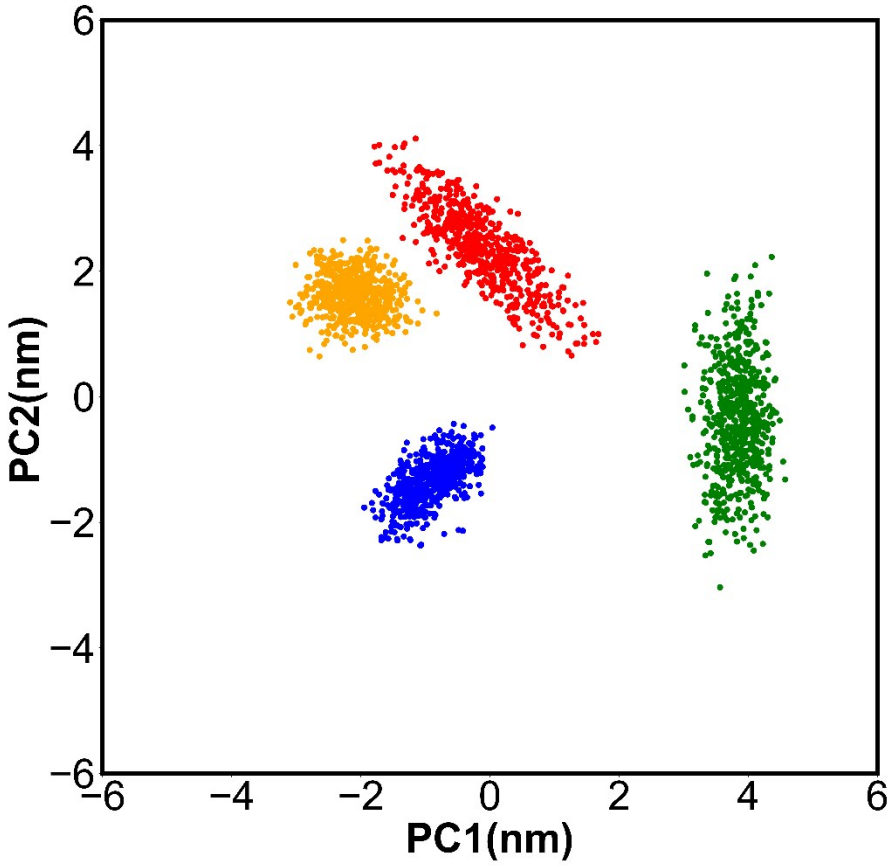

Fig. S3. Principal component analysis (PCA) for Native, P10S, W11R, and K12N MD trajectories. The geometry center position of the native (blue), P10S (red), W11R (orange) and K12N (green) states are (-0.91 nm, -1.34 nm), (-0.12 nm, 2.38 nm), (-2.10 nm, 1.62 nm), and (3.83 nm, -0.39 nm), respectively. The results show that the three different complex states can be separated into three groups (Native; P10S and W11R; K12N) by the first two components.