Insights into phosphorylation-induced influences on conformations and inhibitor

binding of CDK6 through GaMD trajectory-based deep learning

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Fig. S1 Superimposition of the crystal structure and the repaired structure of the inhibitor-CDK6 complex: (A) the 6ZV-bound CDK6; (B) the 6ZZ-bound CDK6 and (C) the 0RS-bound CDK6, in which the crystal structure is shown in green, the repaired structure is shown in blue and the repaired regions are highlighted in red.



Fig. S2 The time course for RMSDs of CDK6.



Fig. S3 The time course of RMSDs for the inhibitors.



Fig. S4 The time course of RGs for CDK6 from six systems.



Fig. S5 Surface area of CDK6: (A) statistic distributions of surface area and (B) the time course of surface area.



Fig. S6 Dynamics cross-correlation maps calculated by using the coordinates of the C α atoms: (A) the 6ZV-bound CDK6; (B) the 6ZV-bound CDK6-pT177; (C) the 6ZZ-bound CDK6; (D) the 6ZZ-bound CDK6-pT177; (E) the 0RS-bound CDK6 and (F) the 0RS-bound CDK6-pT177. The color violet to cyan transformation is used to scale the transformation from the most anti-correlated to the most positively correlated motions.



Fig. S7 Information changes of 6ZV-bound CDK6-pT177 revealed by principal component analysis. The first three PCs (PC1-PC3) show fluctuating regions with 35% of overall fluctuations.



Fig. S8 Information changes of 6ZZ-bound CDK6 revealed by principal component analysis. The first three PCs (PC1-PC3) show fluctuating regions with 51.2% of overall fluctuations.



Fig. S9 Information changes of 6ZZ-bound CDK6-pT177 revealed by principal component analysis. The first three PCs (PC1-PC3) show fluctuating regions with 62.6% of overall fluctuations.



Fig. S10 Information changes of 0RS-bound CDK6 revealed by principal component analysis. The first three PCs (PC1-PC3) show fluctuating regions with 72% of overall fluctuations.



Fig. S11 Information changes of 0RS-bound CDK6-pT177 revealed by principal component analysis. The first three PCs (PC1-PC3) show fluctuating regions with 62.6% of overall fluctuations.