Supplementary Files

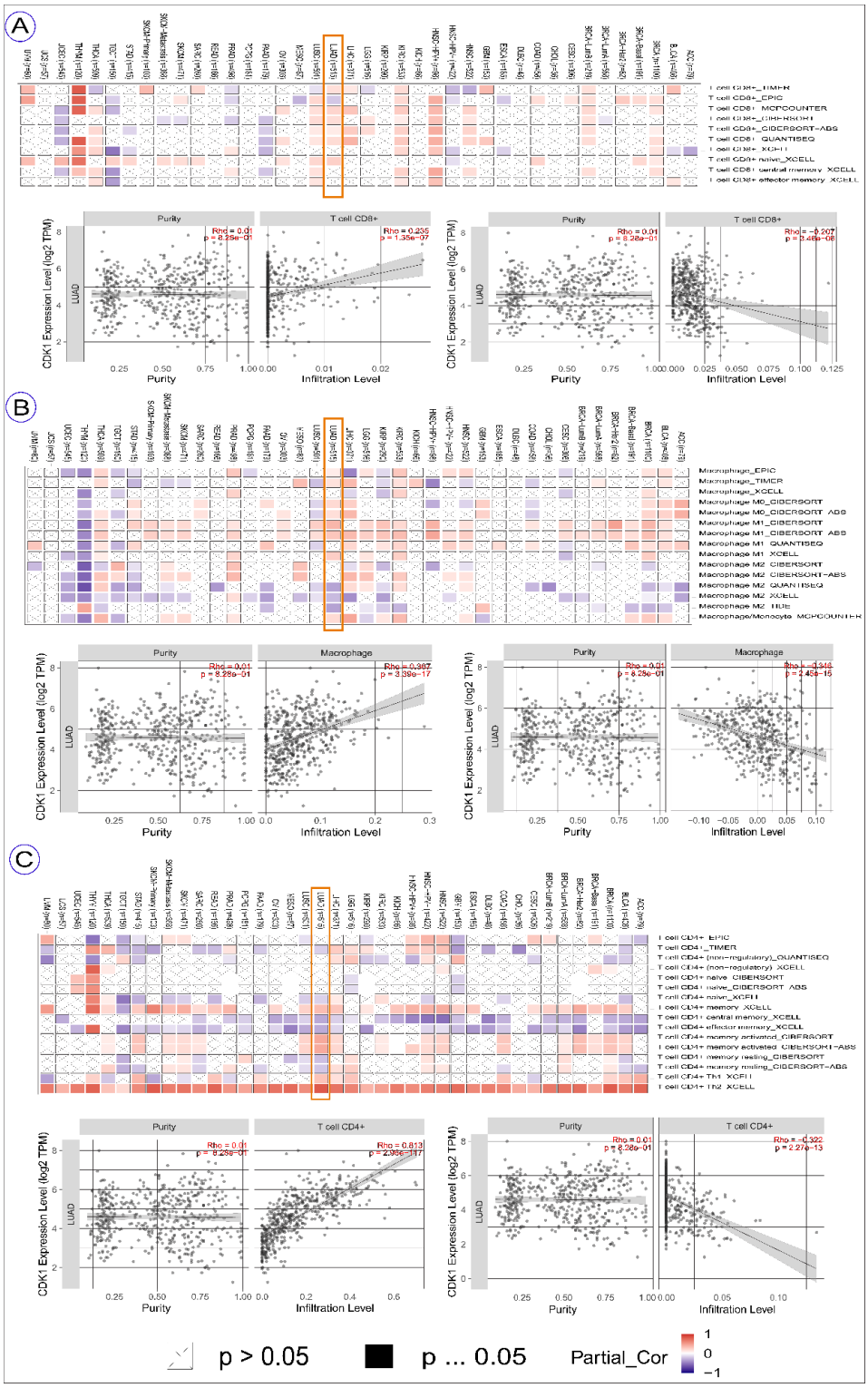

Figure S1. Correlation of CDK1 Expression with Immune Cell Infiltration in LUAD Across CD8+ T Cells (A), Macrophages (B) and CD4+ T Cells (C).

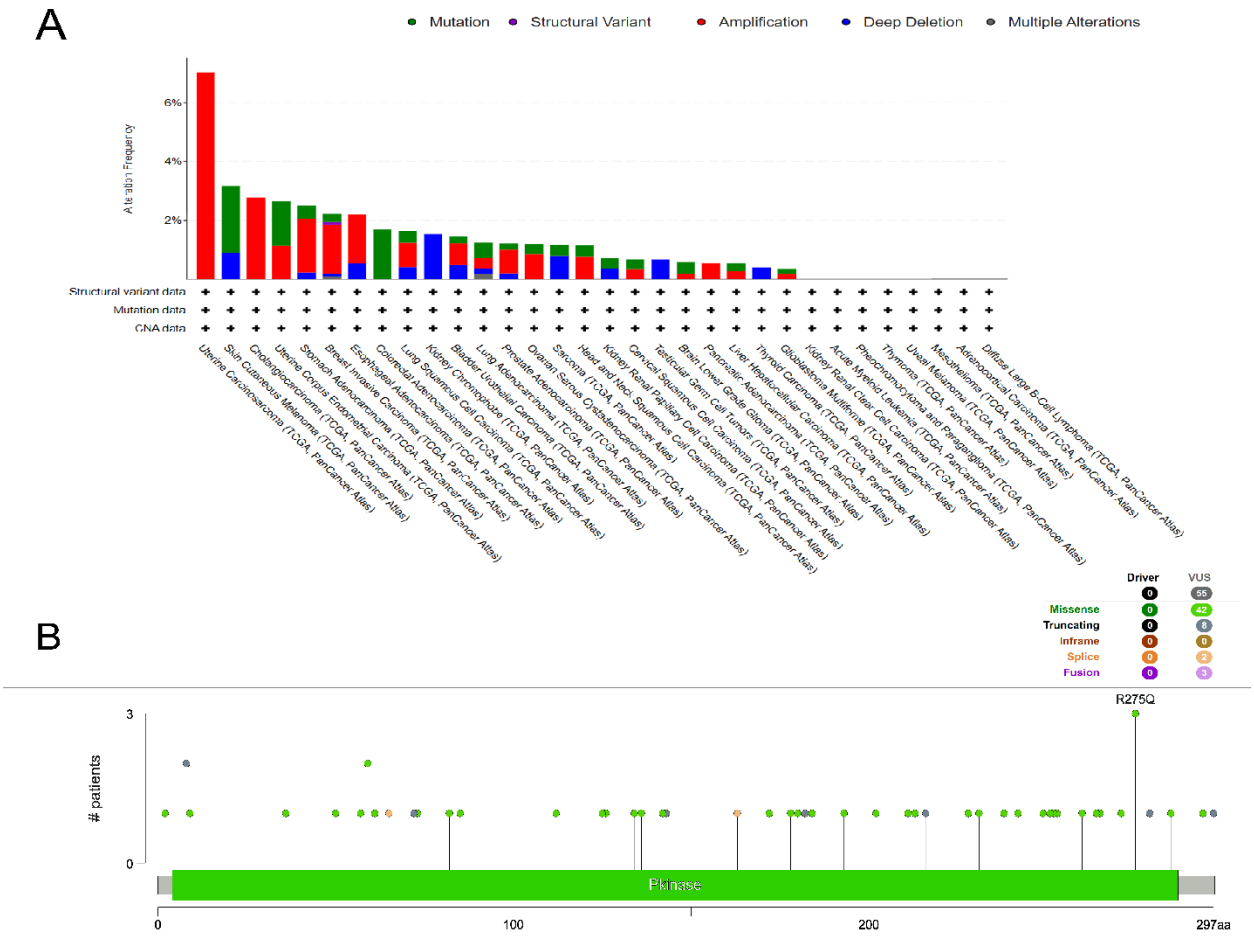

Figure S2. Genetic alterations of CDK1 across cancers. (A) Alteration frequency and types in TCGA datasets. (B) Mutation spectrum and genomic distribution of CDK1 variants.

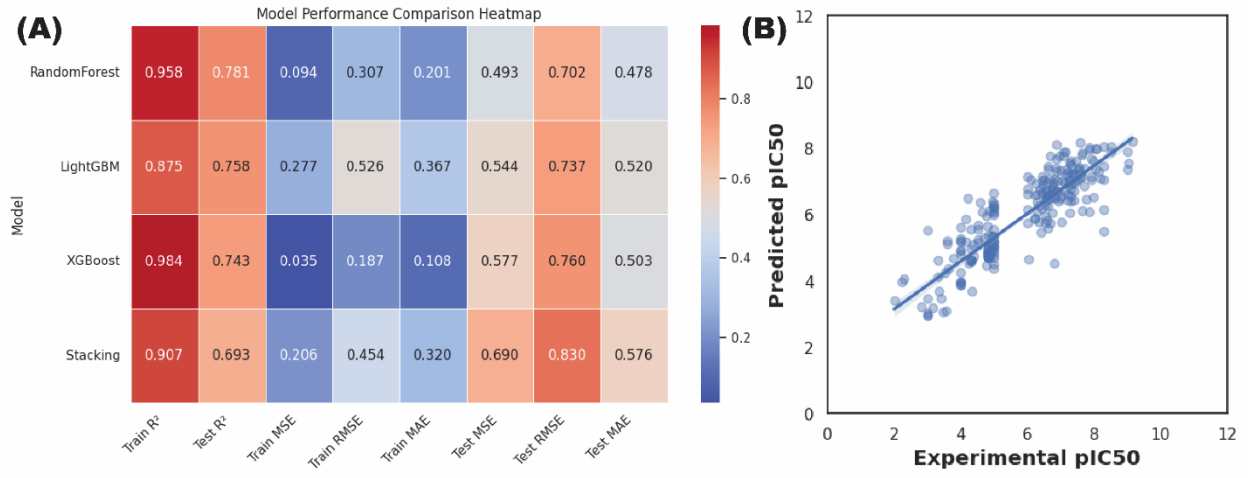

Figure S3. *(A)* Heatmap illustrating the performance of four machine-learning regression models (RandomForest, XGBoost, LightGBM, and Stacking) across training and testing metrics for CDK1 inhibitor prediction. *(B)* Scatter plot showing the correlation between experimentally observed pIC50 values and LightGBM-predicted pIC50 values, demonstrating the model's strong predictive accuracy.

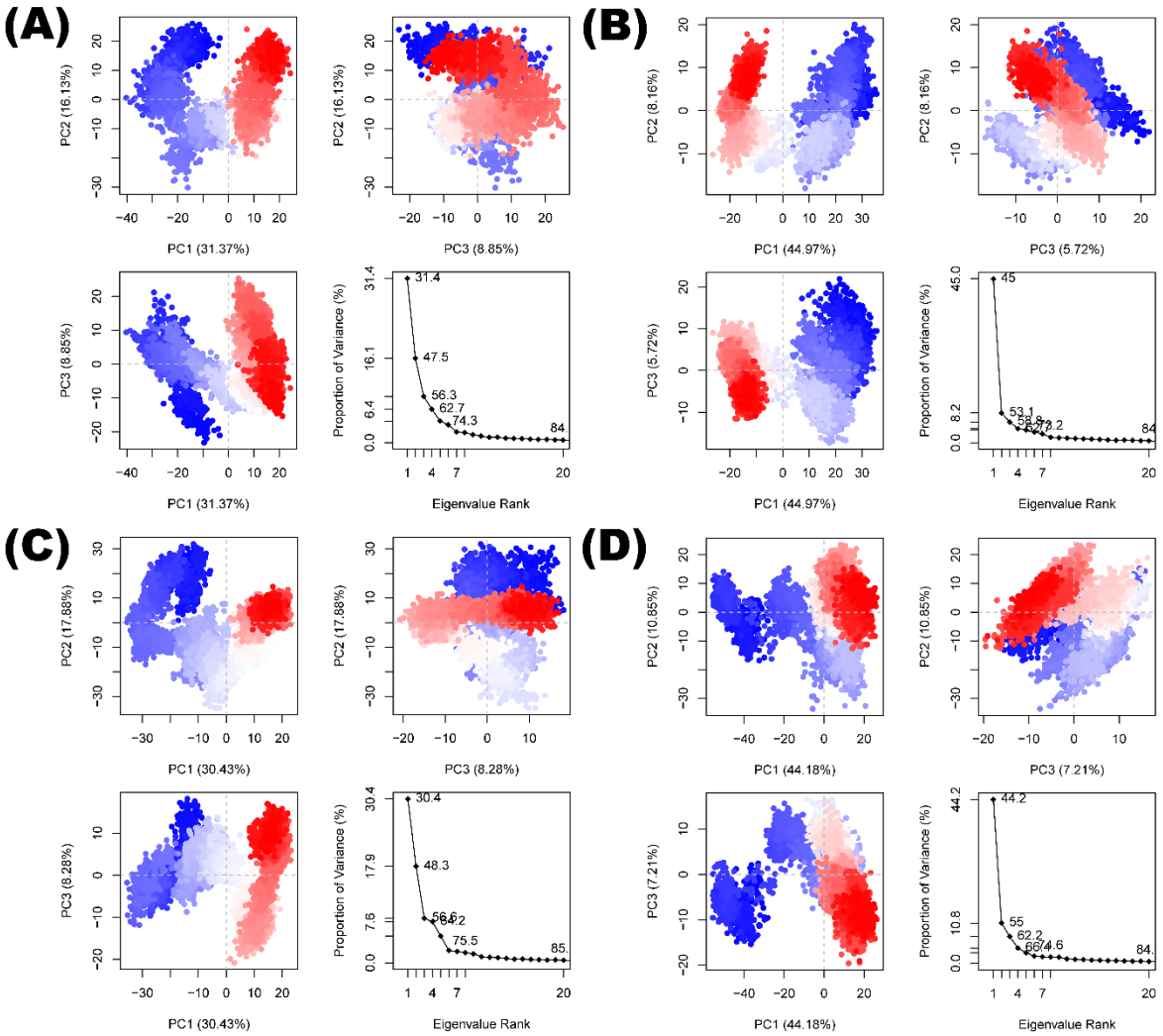

Figure S4. Principal Component Analysis (PCA) Biplots and Scree Plots of CDK1 Complexes: (A) 6GU7_487089, (B) 6GU7_174880, (C) 6GU7_14218027, and (D) Control (AZD5438)

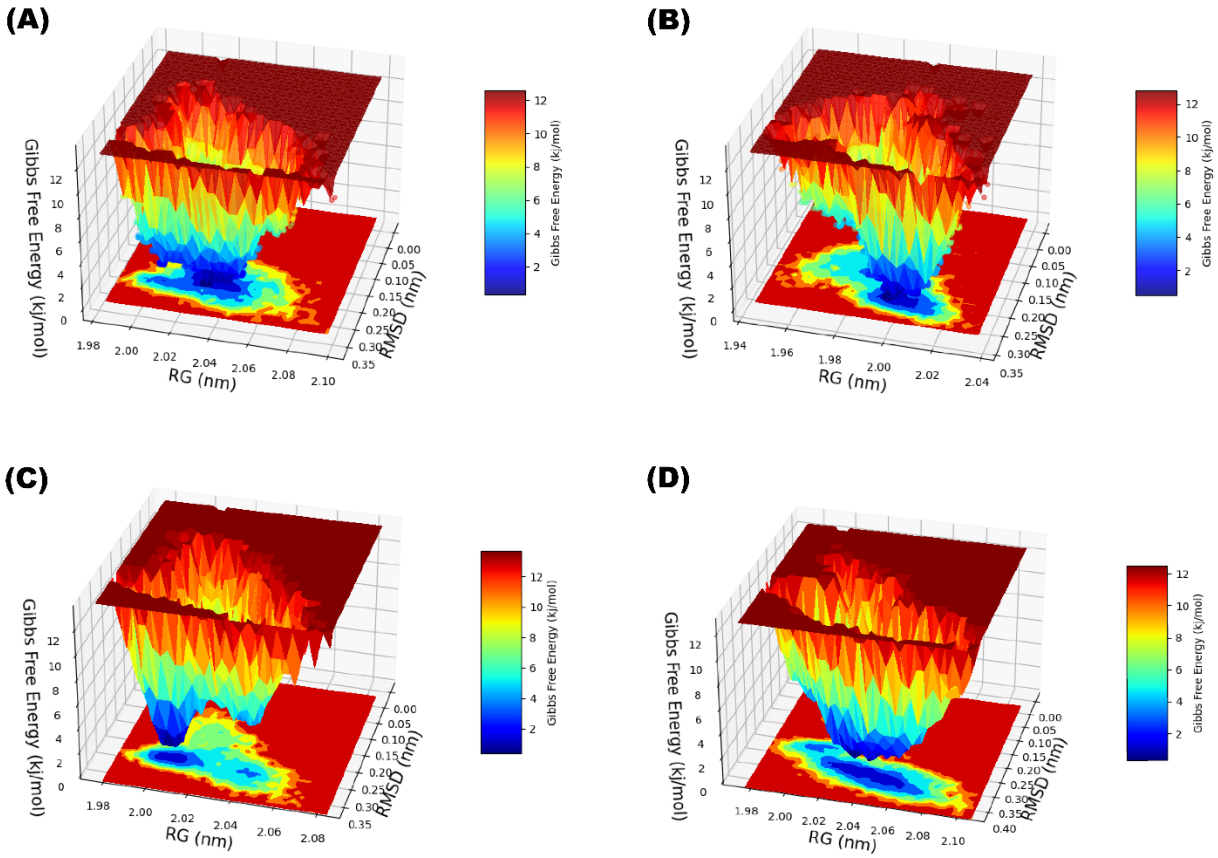

Figure S5. Gibbs Free Energy Landscapes of CDK1-Inhibitor Complexes: (A) 6GU7_487089, (B) 6GU7_174880, (C) 6GU7_14218027, and (D) Control (AZD5438).