

Supplementary Materials:

Table S1. Redocked conformations of co-crystallized ligand with HSV-1 thymidine kinase proteins.

HSV-1 thymidine kinase proteins	Co-crystallized ligands	Binding energy score (kcal/mol)	RMSD value (Å)
1KI7	5-Iododeoxyuridine	-7.285	0.379
1KI4	5-Bromothienyldeoxyuridine	-10.3	0.2
1E2P	6-(dihydroxy-isobutyl)-thymine	-7.318	0.57
1KIM	Deoxythymidine	-9.8	0.3

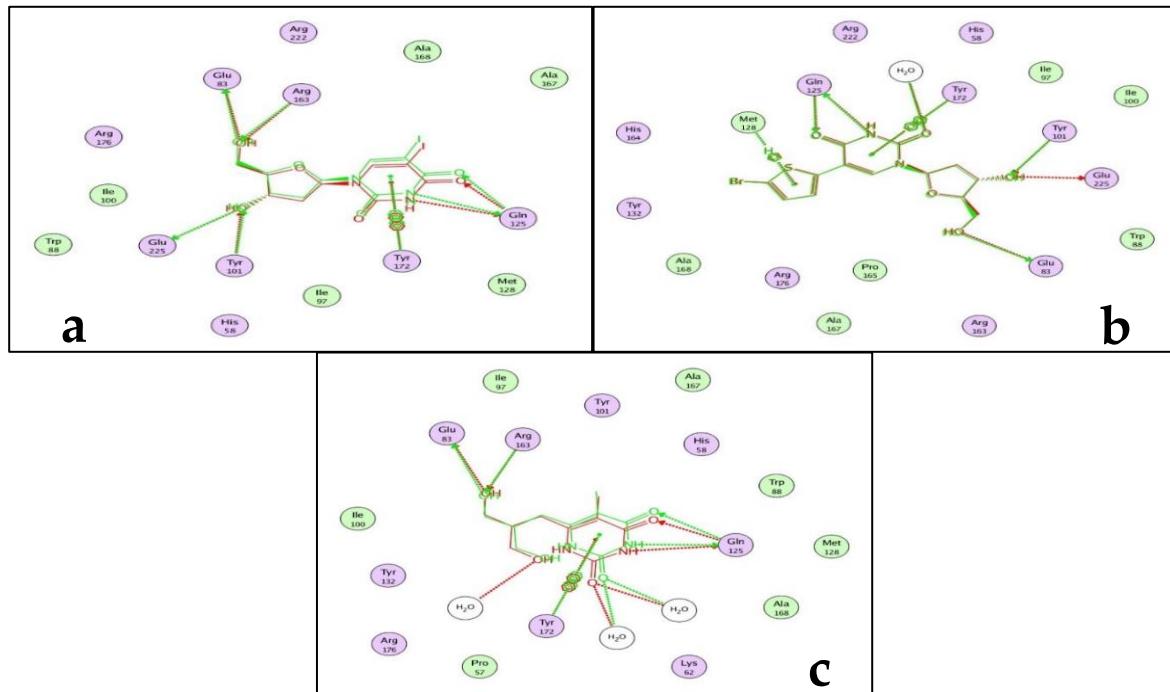


Figure S1. 2D diagram showing superimposition of the co-crystallized ligand (red) and the redocked pose (green) on 1KI7 (A) and 1KI4 (B) and 1E2P (C) thymidine kinase protein.