# Supplementary file 2

Shetty et al., ***BioImpacts.*** 2024;14(4):29951
doi: 10.34172/bi.2023.29951

# Thiazolo-pyridopyrimidines: An *in silico* evaluation as a lead for CDK4/6 inhibition, synthesis and cytotoxicity screening against breast cancer cell lines

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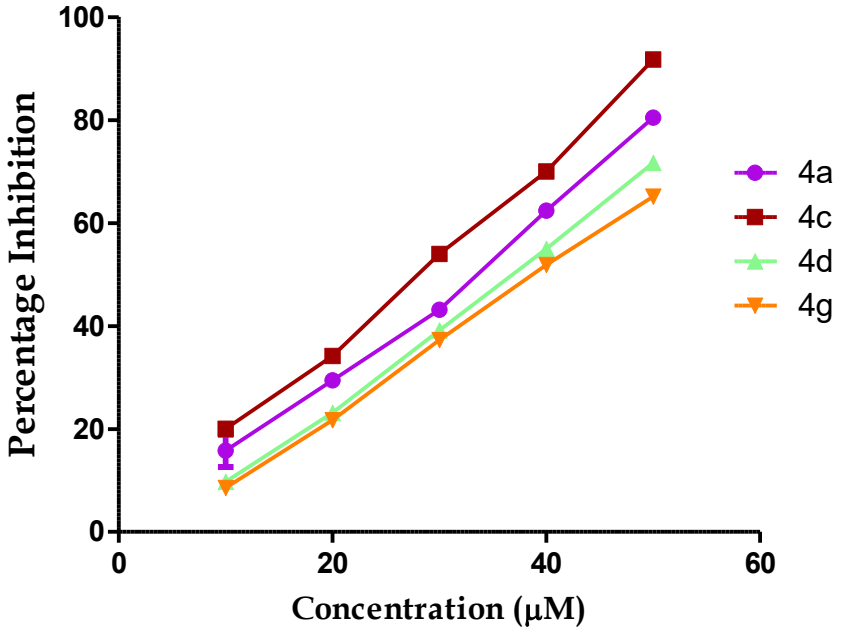

**Fig. S1.** Percentage inhibition against MCF-7 cells by SRB assay

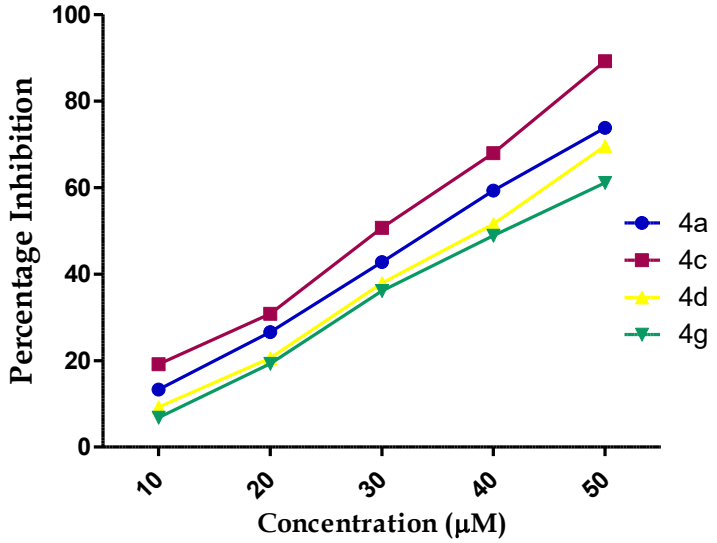


**Fig. S2**. Percentage inhibition against MDAMB-231 cells by SRB assay

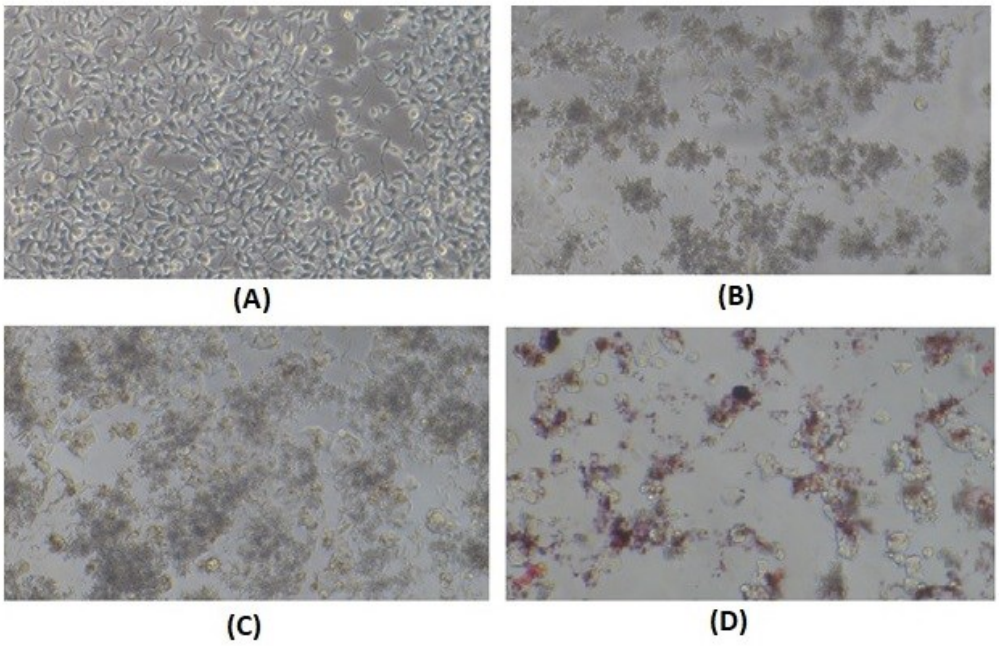


**Fig. S3.** (A) Normal MCF-7 cells. (B) MCF-7 cells after treating with 4a. (C) MCF-7 cells after treating with 4c. (D) MCF-7 after treating with std. doxorubicin

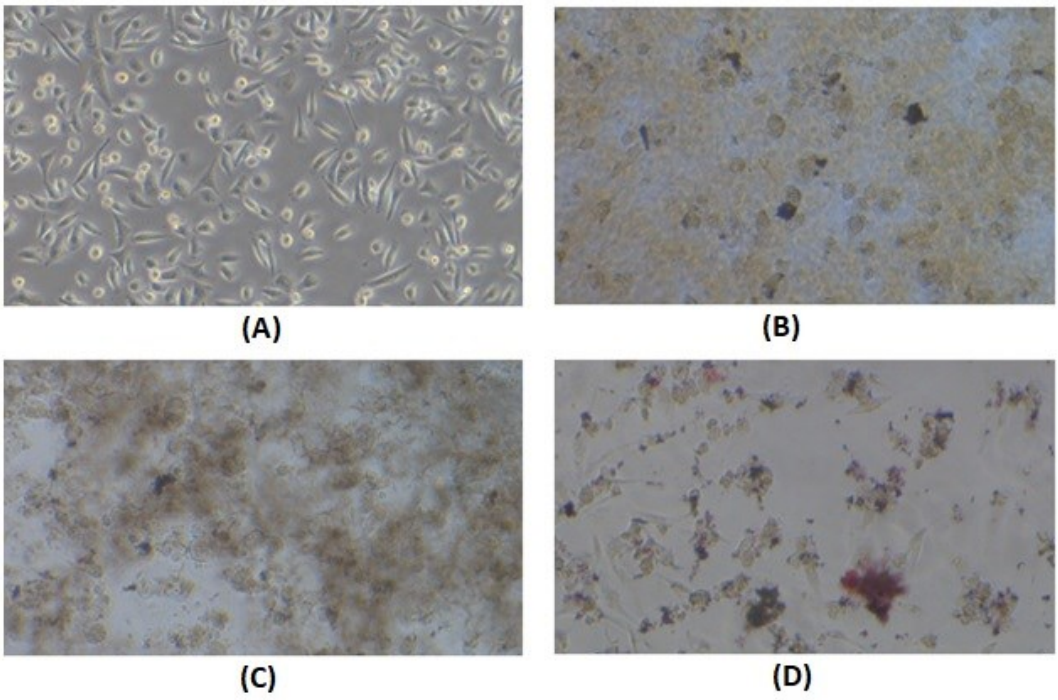


**Fig. S4.** (A) Normal MDA-MB-231 cells. (B) MDA-MB-231 cells after treating with 4a. (C) MDA-MB-231 cells after treating with 4c. (D) MDA-MB-231 after treating with std. doxorubicin.

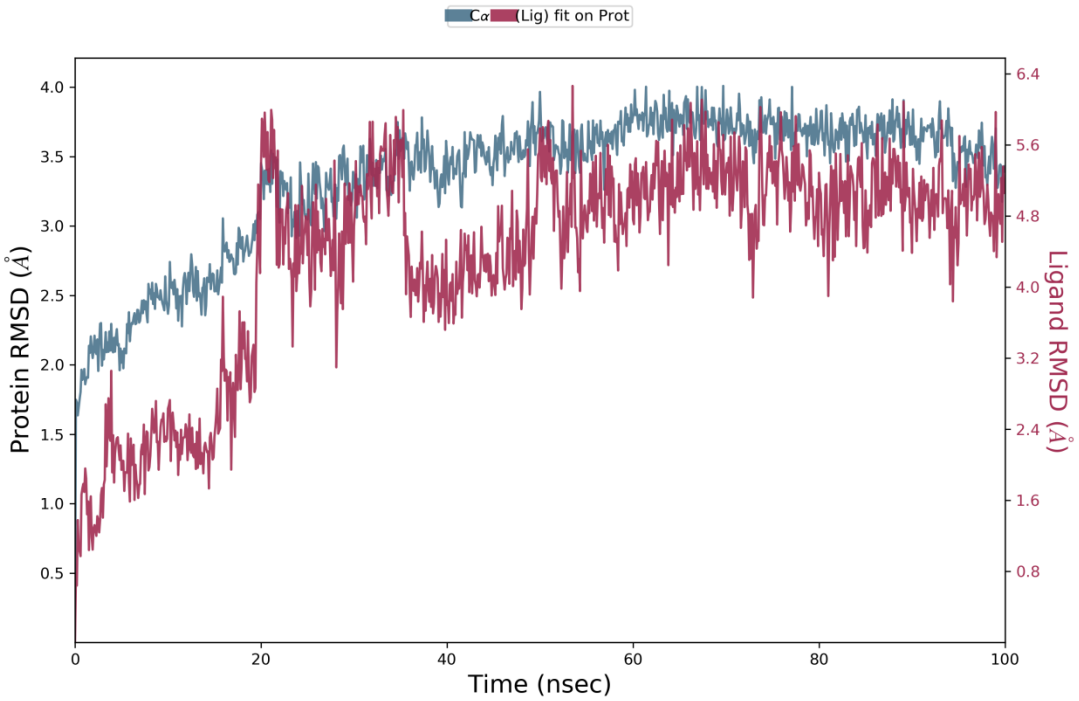


**Fig. S5.** RMSD of backbone atoms comparative to the original 4a-2W96 complex

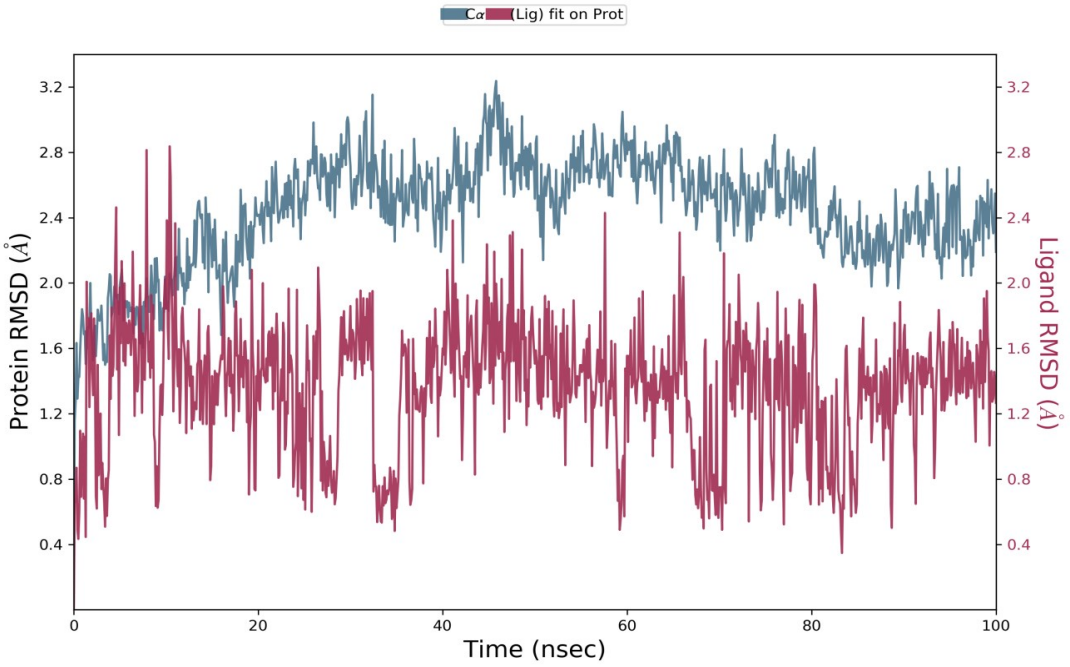


**Fig. S6.** RMSD of backbone atoms comparative to the original 4c-6OQO complex

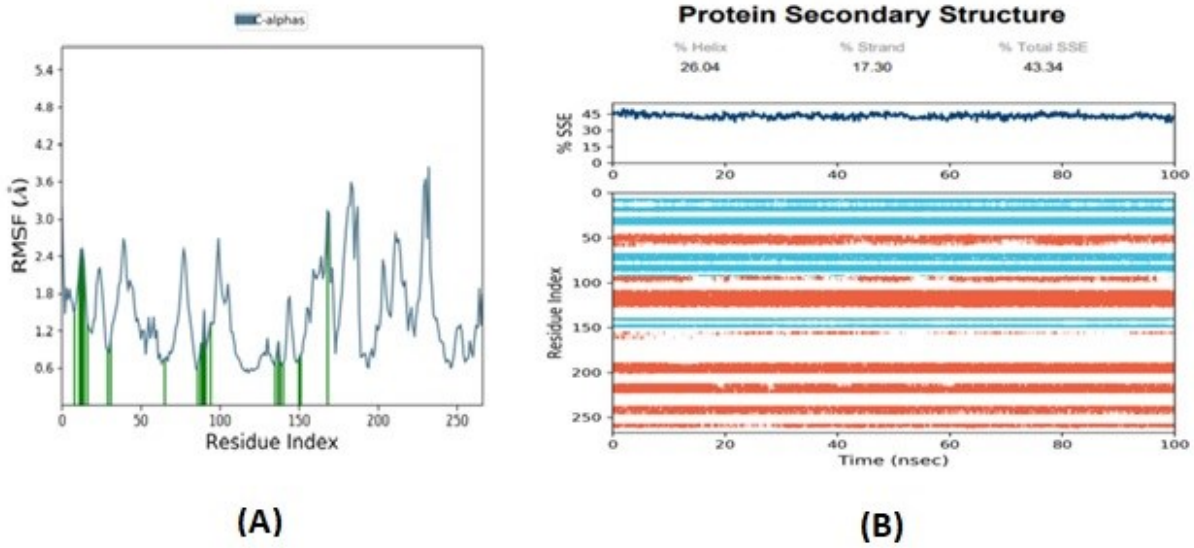


**Fig. S7**. (A) RMSF plot of 2W96 protein in 100 ns simulations. (B) The plot summarizes the secondary structure elements (SSE) composition of 2W96 protein for individual trajectory frame throughout the simulation, and the plot observes each residue and its SSE distribution.

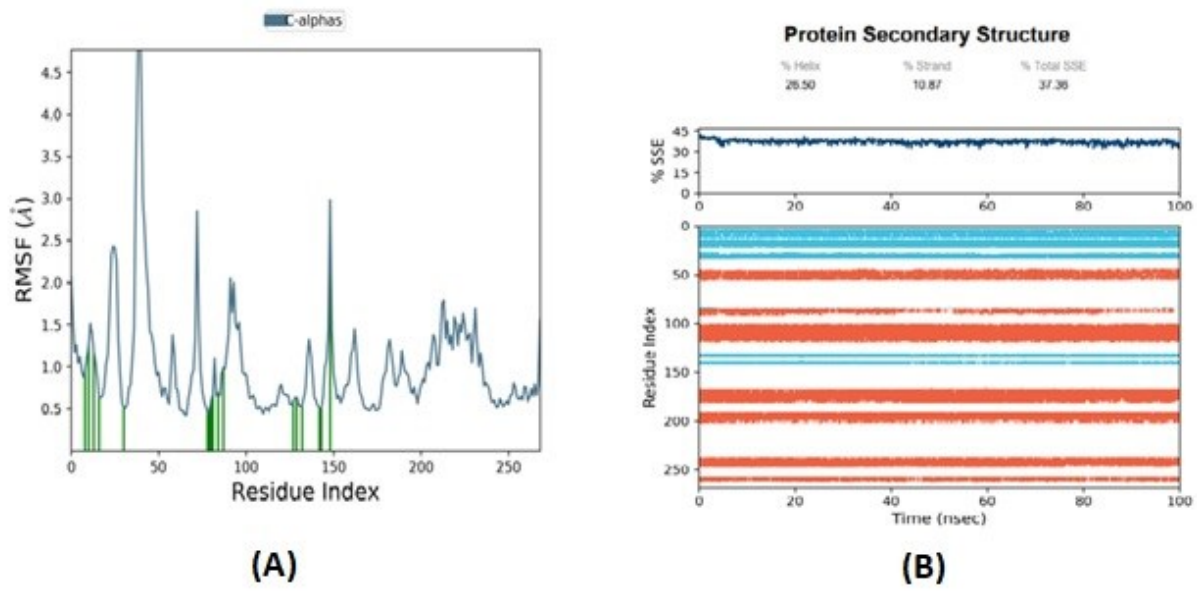


**Fig. S8.** (A) RMSF plot of 6OQO protein in 100 ns simulations. (B) The plot summarizes the secondary structure elements (SSE) composition of 6OQO protein for individual trajectory frame throughout the simulation, and the plot observes each residue and its SSE distribution.

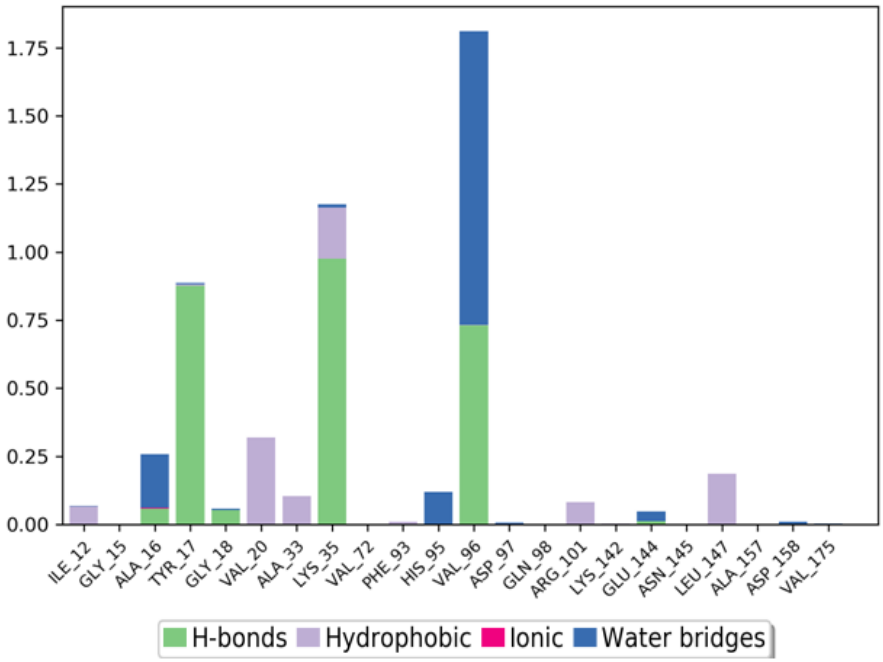


**Fig. S9**. Histogram presentation of pre-residues analysis of 4a in complex with 2W96 protein throughout the 100 ns MD simulations

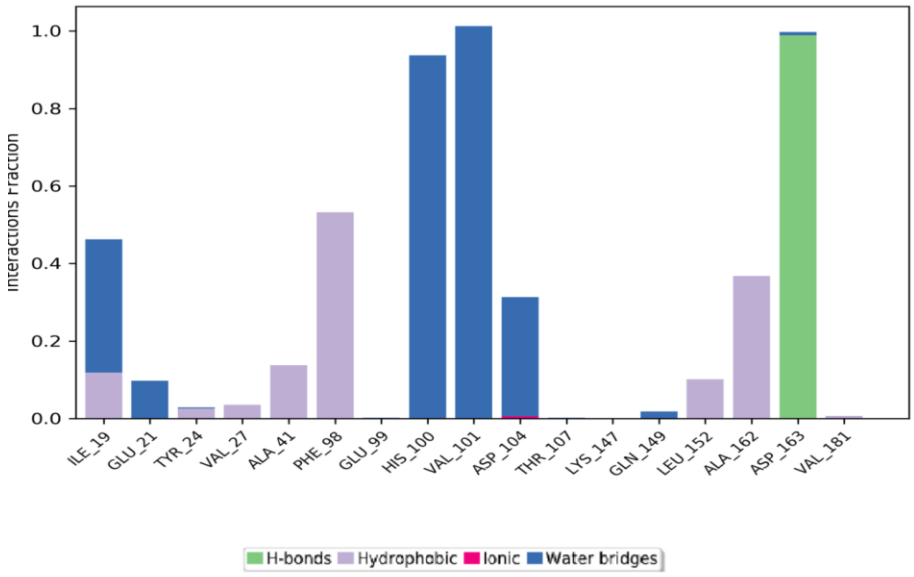


**Fig. S10**. Histogram presentation of pre-residues analysis of 4c in complex with 6OQO protein throughout the 100 ns MD simulations

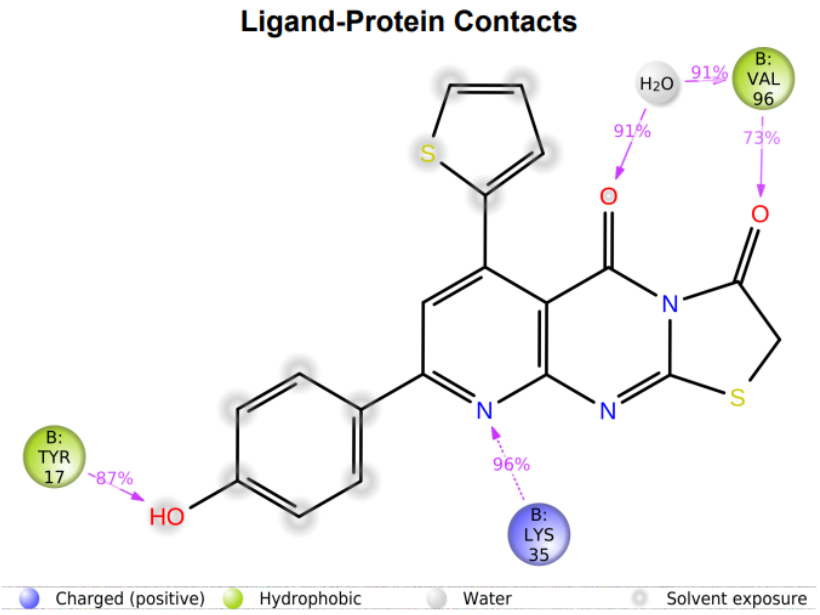


**Fig. S11.** 2D representation of interaction of 4a with 2W96 after simulation

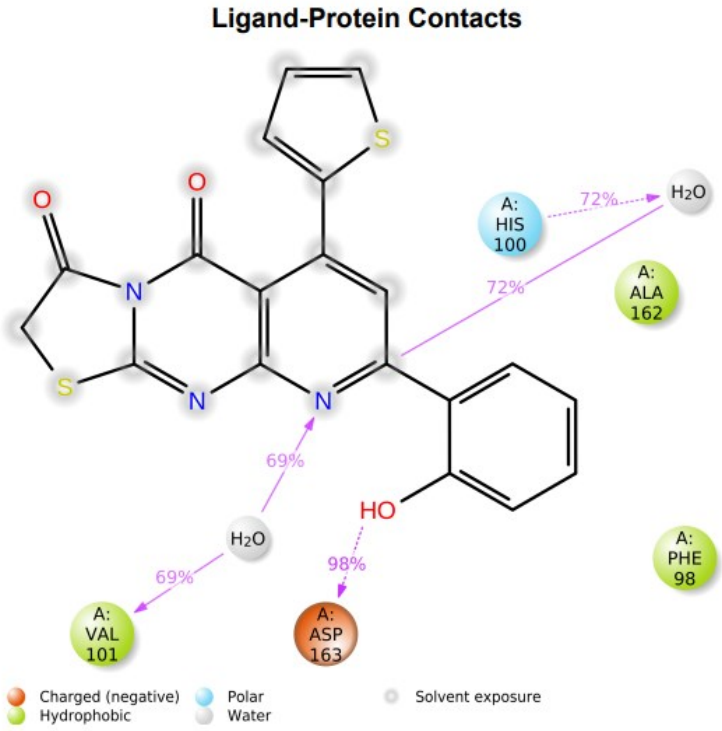


**Fig. S12.** Interaction of 4c with 6OQO after simulation