

GENE	Uniprot ID	PDB ID	ΔG (kcal/mol)	
			5-Fluorouracil	norcantharidin
BCL2A1	Q16548	6vo4	-4.1	-5.2
CA12	O43570	5ll5	-6.1	-6.9
CASP9	P55211	2ar9	-5.5	-7.1
CES1	P23141	5a7g	-5.2	-6.1
CYP19A1	P11511	3s79	-5.1	-5.4
CYP1A2	P05177	2hi4	-5.7	-6.2
PTGS1	P23219	6y3c	-6.2	-6.8
SIRT2	Q8IXJ6	5y5n	-5.0	-5.5

Table S1. Molecular docking results of 8 key expressed proteins.

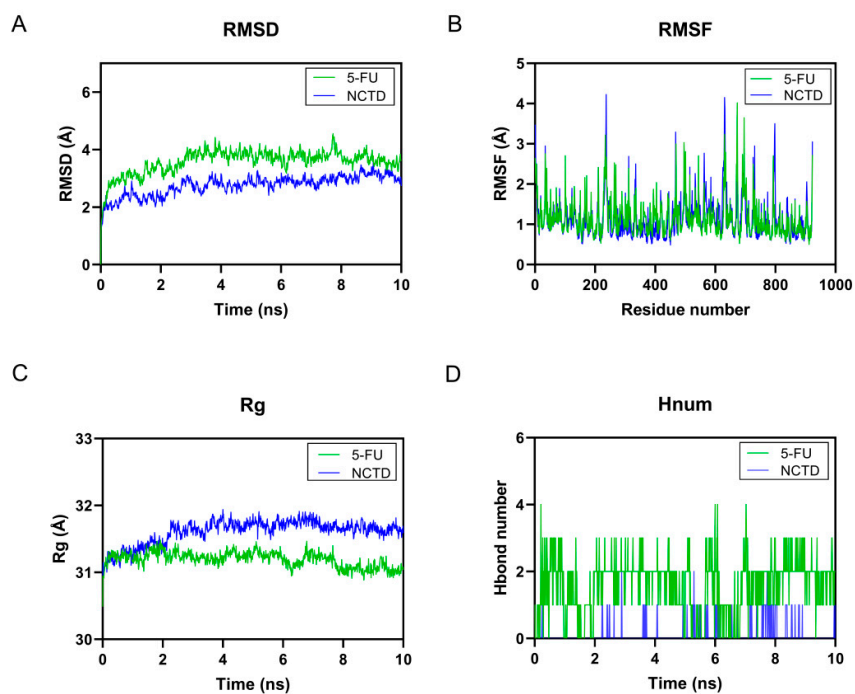


Figure S1. Molecular Dynamics Simulation results of caspase-9-5-FU complex and caspase-9-NCTD complex, respectively. (A) Root Mean Square Deviation. (B) Root Mean Square Fluctuation. (C) Radius of Gyration. (D) The number of hydrogen bonds.