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Bioinformatic analysis of cervical cancer-associated hub genes and repurposing of 5-fluorouracil and gemcitabine as potential therapeutic agents

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Supplementary Data

Table 1 — The DEGs in GO analysis both upregulated and downregulated for GSE26511

Sl. No	Particulars	No. of genes in the dataset	Fold enrichment	P-value (Hypergeometric test)	Q-value (Storey-Tibshirani method)	Genes mapped (from input data set)
1	Plasma membrane	14	1.4290437	0.090818	1	SDK2; GHR; ITSN1; SLC12A2; PARVA; SDK1; SLC6A6; FGF2; ADD3; CLIC4; SLC1A4; APP; EPM2A; SLC4A7;
2	Nucleus	20	1.2144407	0.166914	1	ID4; EBF1; BACH2; ITSN1; TCF4; FMNL2; FAM188A; CLK1; PARVA; RBPJ; FGF2; IGFBP5; ADD3; CLIC4; WWTR1; APP; NR2F1; EPM2A; IL33; TNPO1;
3	Cytosol	8	2.4129404	0.015536	1	TKT; ITSN1; TCF4; CTNNAL1; PARVA; UGDH; CLIC4; EPM2A;
4	Cytoplasm	22	1.3741314	0.040709	1	ID4; BACH2; TKT; ITSN1; FMNL2; GUCY1A3; TPSAB1; FAM188A; CTNNAL1; CLK1; PARVA; SRR; CEP68; IGFBP5; ADD3; CLIC4; SLC1A4; WWTR1; APP; ARHGAP12; EPM2A; TNPO1;
5	Exosomes	7	1.2176167	0.351047	1	TKT; ITSN1; SLC12A2; UGDH; CLIC4; SLC1A4; APP;
6	Extracellular	10	1.9463991	0.027131	1	GHR; LTBP2; PTN; TKT; TPSAB1; SLC12A2; FGF2; IGFBP5; APP; FST;
Cellular component downregulated						
1	Plasma membrane	8	0.9851969	0.586518	1	RAET1E; SGCD; MPP5; RALBP1; RAB27B; SHANK2; STIM2; NGEF;
2	Integral to membrane	3	0.7567468	0.776775	1	ADGRF4; GALNT3; CNIH4;
3	Nucleus	19	1.3912157	0.046305	1	NR2F1; CDKN2B; HDAC5; BORA; RBPJ; ZNF550; PRR11; BNC2; LPIN1; ID2; MED14; HELQ; MPP5; RALBP1; RAB27B; ZNF398; STIM2; CASP14; HIST1H4H;

4	Cytoplasm	16	1.2052654	0.215979	1	SOCS6; CDKN2B; HDAC5; CCM2; BORA; SGCD; ACOT8; NDFIP2; MPP5; RALBP1; RAB27B; SHANK2; ZNF398; CASP14; NGEF; HIST1H4H;
5	Exosomes	4	0.8398855	0.722489	1	GALNT3; MPP5; RAB27B; HIST1H4H;
6	Endoplasmic reticulum	4	1.5542381	0.255562	1	CNIH4; TPST2; NDFIP2; STIM2;
Molecular function upregulated						
1	Molecular function unknown	9	0.667886	0.954181	1	FILIP1L; PRR5L; OGFRL1; FMNL2; FAM188A; CTNNAL1; CEP68; EPM2AIP1; IL33;
2	Cell adhesion molecule activity	3	3.5629778	0.052068	1	SDK2; SDK1; IGFBP5;
3	Transporter activity	4	2.9337504	0.046946	1	SLC6A6; SLC1A4; SLC4A7; TNPO1;
4	Transcription regulator activit	3	1.5245679	0.316003	1	ID4; RBPJ; WWTR1;
5	Receptor activity	2	2.3463113	0.21101	1	GHR; APP;
6	Transcription factor activity	4	2.0069471	0.137832	1	EBF1; BACH2; TCF4; RBPJ;
Molecular function downregulated						
1	Molecular function unknown	9	0.73637	0.904529	1	CCM2L; CCM2; BORA; C1orf131; CNIH4; PRR11; LPIN1; MPP5; ASB7;
2	Cell adhesion molecule activity	2	2.623229	0.178103	1	SGCD; STIM2;
3	Transporter activity	4	3.234571	0.03451	1	NDFIP2; SLC35D2; NIPSNAP3B; SLC25A43;
4	Transcription regulator activity	5	2.797767	0.031866	1	HDAC5; RBPJ; ID2; MED14; ZNF398;
5	Transcription factor activity	2	1.109127	0.546618	1	RBPJ; BNC2;
6	Receptor signalling complex scaffold activity	2	2.900207	0.152232	1	SOCS6; CCM2;
Biological Process upregulated						
1	Biological process unknown	7	0.62438	0.95592	1	FILIP1L; PRR5L; OGFRL1; FMNL2; CEP68; EPM2AIP1; IL33;
2	Cell growth and/or maintenance	4	1.50201	0.276553	1	LTBP2; PARVA; SDK1; ADD3;
3	Transport	6	2.084392	0.065478	1	SLC12A2; SLC6A6; CLIC4; SLC1A4; SLC4A7; TNPO1;
4	Cell communication	11	1.249528	0.254235	1	SDK2; GHR; PTN; GUCY1A3; FGF2; IGFBP5; APP; ARHGAP12; FST; NR2F1; EPM2A;
5	Signal transduction	13	1.393563	0.122315	1	SDK2; GHR; PTN; ITSN1; GUCY1A3; CLK1; FGF2; IGFBP5; APP; ARHGAP12; FST; NR2F1; EPM2A;
6	Regulation of nucleobase, nucleoside, nucleotide and nucleic acid metabolism	6	0.895526	0.681134	1	ID4; EBF1; BACH2; TCF4; RBPJ; WWTR1;
Biological Process downregulated						
1	Biological process unknown	6	0.5902	0.962859	1	CCM2L; CCM2; C1orf131; CNIH4; PRR11; LPIN1;
2	Protein metabolism	2	0.705848	0.788548	1	GALNT3; CASP14;

3	Transport	4	1.533356	0.263977	1	NDFIP2; SLC35D2; NIPSNAP3B; SLC25A43;
4	Cell communication	12	1.502779	0.085897	1	ADGRF4; NR2F1; SOCS6; CDKN2B; CCM2; SGCD; MPP5; RALBP1; ASB7; RAB27B; STIM2; NGEF;
5	Signal transduction	12	1.418358	0.121004	1	ADGRF4; NR2F1; SOCS6; CDKN2B; CCM2; SGCD; MPP5; RALBP1; ASB7; RAB27B; STIM2; NGEF;
6	Regulation of nucleobase, nucleoside, nucleotide and nucleic acid metabolism	10	1.644491	0.071975	1	HDAC5; RBPJ; ZNF550; BNC2; ID2; MED14; HELQ; ZNF398; TDRKH; HIST1H4H;

Cellular component upregulated

Sl. No	Particulars	No. of genes in the dataset	Fold enrichment	P-value (Hypergeometric test)	Q-value (Storey-Tibshirani method)	Genes mapped (from input data set)
1	Nucleus	17	1.1757099	0.242558	1	FBXO5; GEMIN4; MYC; CDKN1B; LUZP1; SKP2; IMP3; TRIM32; HJURP; RRS1; MTPAP; GNAI2; DDX20; IQGAP1; TP53RK; TP53; NR2F2;
2	Cytosol	9	3.0910464	0.001838	1	FBXO5; GEMIN4; CDKN1B; FADD; AMD1; CENPL; GNAI2; DDX20; TP53;
3	Cytoplasm	15	1.067224	0.43557	1	FBXO5; GEMIN4; DNAAF2; CDKN1B; FADD; LUZP1; FZD2; AMD1; TRIM32; HJURP; GNAI2; DDX20; FBXL5; IQGAP1; TP53;
4	Exosomes	5	0.9910531	0.583057	1	GEMIN4; RHOB; LUZP1; GNAI2; IQGAP1;
5	Endoplasmic reticulum	5	1.8339793	0.13373	1	LPCAT1; GAS1; EDEM3; GNAI2; TP53;
6	Extracellular	5	0.445103	0.950673	1	ADAMTS15; MFAP5;

Cellular component downregulated

1	Plasma membrane	4	0.4791256	0.980852	1	SLC30A1; ENAH; SULF2; BICD1;
2	Nucleus	20	1.4225711	0.031407	1	HSPA6; ATF3; GADD45B; TRIB3; NDRG1; PPP1R15A; ZFAND2A; DNAJB1; ENAH; ASS1; RBM33; MAFK; MAF; SERTAD2; SKIL; SPINK4; ETS1; MT1F; BNIP3L; BCL2;
3	Cytosol	8	2.8264692	0.005884	1	HMOX1; DNAJB1; ENAH; EGLN1; ASS1; AKR1C1; SARS; BCL2;
4	Cytoplasm	22	1.6096295	0.003703	1	HSPA6; TRIB3; NDRG1; ZFAND2A; DNAJB1; ENAH; SULF2; EGLN1; AKR1C1; RBM33; VEGFA; MAF; SERTAD2; SKIL; SPINK4; ALDH1A3; FHL1; ETS1; MT1F; SARS; BNIP3L; BCL2;

5	Endoplasmic reticulum	9	3.3924425	0.000936	1	HSPA6; HMOX1; PPP1R15A; DNAJB1; ALDH3A2; SEC24A; BNIP3L; BCL2; GDF15;
6	Extracellular	6	1.3688944	0.270688	1	SULF2; C2; VEGFA; SPINK4; ETS1; GDF15;
			Molecular function upregulated			
1	Molecular function unknown	18	1.335031	0.095328	1	FBXO5; GEMIN4; DNAAF2; FAM83D; GAS1; FAM217B; TMEM60; TMCC1; SMG8; FASTKD3; KBTBD6; CENPL; C2orf69; HJURP; RRS1; MN1; KBTBD7; ARMCX2;
2	Transcription regulator activity	2	1.018067	0.593454	1	LUZP1; TRIM32;
3	Transcription factor activity	2	1.005976	0.60008	1	MYC; TP53;
4	Ubiquitin-specific protease activity	2	2.246736	0.22499	1	SKP2; FBXL5;
5	GTPase activity	2	3.815332	0.097302	1	RHOB; GNAI2;
6	Ribonucleoprotein	2	20.65452	0.004251	1	IMP3; RRS1;
			Molecular function downregulated			
1	Molecular function unknown	10	0.79765	0.851226	1	GADD45B; KDM7A; NDRG1; PPP1R15A; FEM1C; AZIN1; SKIL; HECA; FHL1; DOCK11;
2	Transporter activity	4	3.153727	0.037414	1	BICD1; CHMP1B; MT1F; SEC24A;
3	Catalytic activity	6	5.117577	0.001021	1	HMOX1; SULF2; ALDH3A2; ASS1; AKR1C1; ALDH1A3;
4	Transcription factor activity	3	1.619418	0.28398	1	MAFK; MAF; ETS1;
5	RNA binding	2	2.487785	0.193176	1	ZFAND2A; RBM33;
6	Heat shock protein activity	2	33.71174	0.00161	1	HSPA6; DNAJB1;
			Biological Process upregulated			
1	Biological_process unknown	13	1.1587995	0.320961	1	DNAAF2; FAM83D; FAM217B; TMEM60; TMCC1; SMG8; FASTKD3; KBTBD6; CENPL; C2orf69; HJURP; RRS1; KBTBD7;
2	Metabolism	5	1.2543995	0.369546	1	TRMT5; MGAT2; EDEM3; AMD1; DDX20;

3	Energy pathways	4	1.0347618	0.550143	1	TRMT5; MGAT2; EDEM3; DDX20;
4	Cell communication	11	1.2495282	0.254235	1	FBXO5; CDKN1B; GAS1; RHOB; FADD; FZD2; GNAI2; MN1; IQGAP1; TP53RK; NR2F2;
5	Signal transduction	11	1.1793337	0.322835	1	FBXO5; CDKN1B; GAS1; RHOB; FADD; FZD2; GNAI2; MN1; IQGAP1; TP53RK; NR2F2;
6	Regulation of nucleobase, nucleoside, nucleotide and nucleic acid metabolism	6	0.8955264	0.681134	1	MYC; LUZP1; IMP3; TRIM32; MTPAP; TP53;
Biological Process downregulated						
1	Metabolism	8	2.155915	0.028461	1	HMOX1; SULF2; ALDH3A2; ASS1; AKR1C1; AZIN1; ALDH1A3; SARS;
2	Energy pathways	7	1.944531	0.064023	1	HMOX1; SULF2; ASS1; AKR1C1; AZIN1; ALDH1A3; SARS;
3	Transport	5	1.867857	0.127237	1	SLC30A1; BICD1; CHMP1B; MT1F; SEC24A;
4	Cell communication	8	0.97722	0.592991	1	GADD45B; TRIB3; NDRG1; PPP1R15A; VEGFA; SKIL; DOCK11; GDF15;
5	Signal transduction	9	1.037469	0.513288	1	GADD45B; TRIB3; NDRG1; PPP1R15A; ZFAND2A; VEGFA; SKIL; DOCK11; GDF15;
6	Regulation of nucleobase, nucleoside, nucleotide and nucleic acid metabolism	5	0.802495	0.769525	1	ATF3; RBM33; MAFK; SERTAD2; ETS1;

Table 2 — The DEGs in GO analysis both upregulated and downregulated for GSE1827

Sl. No	Particulars	No. of genes in the dataset	Fold enrichment	P-value (Hypergeometric test)	Q-value (Storey-Tibshirani method)	Genes mapped (from the input data set)
1	Transmembrane transport of small molecules	4	3.0316033	0.039696	1	SLC12A2; SLC6A6; SLC1A4; SLC4A7;
2	Transport of inorganic cations/anions and amino acids/oligopeptides	4	12.189941	0.000278	1	SLC12A2; SLC6A6; SLC1A4; SLC4A7;
3	SLC-mediated transmembrane transport	4	4.6393927	0.009712	1	SLC12A2; SLC6A6; SLC1A4; SLC4A7;

4	Glypican pathway	5	1.0724684	0.514741	1	ITSN1; TCF4; FGF2; APP; FST;
5	Glypican 1 network	5	1.1047415	0.48577	1	ITSN1; TCF4; FGF2; APP; FST;
6	Proteoglycan syndecan-mediated signaling events	5	1.0668743	0.519892	1	PTN; ITSN1; TCF4; FGF2; FST;
The downregulated DEGs in the KEGG pathway analysis of GSE26511						
1	Syndecan-1-mediated signaling events	3	0.7678783	0.783197	1	CDKN2B; CCM2; ID2;
2	Regulation of CDC42 activity	5	2.1584404	0.072547	1	CDKN2B; CCM2; ID2; RALBP1; NGEF;
3	Glypican pathway	3	0.7460212	0.801172	1	CDKN2B; CCM2; ID2;
4	GMCSF-mediated signaling events	3	0.772644	0.779264	1	CDKN2B; CCM2; ID2;
5	CDC42 signaling events	5	2.1956052	0.068313	1	CDKN2B; CCM2; ID2; RALBP1; NGEF;
6	Signaling events mediated by Hepatocyte Growth Factor Receptor (c-Met)	3	0.772045	0.779759	1	CDKN2B; CCM2; ID2;

Table 3 — The DEGs in the KEGG pathway analysis both upregulated and downregulated for GSE26511

Sl. No	Particulars	No. of genes in the dataset	Fold enrichment	P-value (Hypergeometric test)	Q-value (Storey-Tibshirani method)	Genes mapped (from the input data set)
1	Metabolism	7	2.4341324	0.018445	1	GEMIN4; SKP2; SMG8; NT5C1B-RDH14; AMD1; DDX20; IQGAP1;
2	Syndecan-1-mediated signaling events	6	1.324227	0.292509	1	MYC; CDKN1B; SKP2; GNAI2; IQGAP1; TP53;
3	Glypican pathway	7	1.5005995	0.167705	1	MYC; CDKN1B; SKP2; FZD2; GNAI2; IQGAP1; TP53;
4	TRAIL signaling pathway	7	1.5119247	0.162894	1	MYC; CDKN1B; FADD; SKP2; GNAI2; IQGAP1; TP53;
5	Sphingosine 1-phosphate (S1P) pathway	7	1.5315749	0.154883	1	MYC; CDKN1B; FADD; SKP2; GNAI2; IQGAP1; TP53;
6	Proteoglycan syndecan-mediated signaling events	7	1.4927723	0.171114	1	MYC; CDKN1B; SKP2; FZD2; GNAI2; IQGAP1; TP53;

Table 4 — The DEGs in the KEGG pathway analysis both upregulated and downregulated for GSE41827

The downregulated DEGs in the KEGG pathway analysis of GSE41827

1	Syndecan-1-mediated signaling events	14	2.716642	0.000104	0.028946603	ATF3; HMOX1; GADD45B; NDRG1; PPP1R15A; ENAH; EGLN1; VEGFA; MAF; SKIL; ETS1; BNIP3L; BCL2; GDF15;
2	Glypican pathway	14	2.639315	0.000145	0.034856455	ATF3; HMOX1; GADD45B; NDRG1; PPP1R15A; ENAH; EGLN1; VEGFA; MAF; SKIL; ETS1; BNIP3L; BCL2; GDF15;
3	GMCSF-mediated signaling events	14	2.733503	0.000097	0.028946603	ATF3; HMOX1; GADD45B; NDRG1; PPP1R15A; ENAH; EGLN1; VEGFA; MAF; SKIL; ETS1; BNIP3L; BCL2; GDF15;
4	Nectin adhesion pathway	14	2.727156	0.0000999	0.028946603	ATF3; HMOX1; GADD45B; NDRG1; PPP1R15A; ENAH; EGLN1; VEGFA; MAF; SKIL; ETS1; BNIP3L; BCL2; GDF15;
5	TRAIL signaling pathway	14	2.659234	0.000133	0.032754311	ATF3; HMOX1; GADD45B; NDRG1; PPP1R15A; ENAH; EGLN1; VEGFA; MAF; SKIL; ETS1; BNIP3L; BCL2; GDF15;
6	IGF1 pathway	14	2.735625	0.000096	0.028946603	ATF3; HMOX1; GADD45B; NDRG1; PPP1R15A; ENAH; EGLN1; VEGFA; MAF; SKIL; ETS1; BNIP3L; BCL2; GDF15;

Table 5 — Molinspiration property of the four drugs

Compound	miLogP	natoms	nON	nOHNH	nrotb
Ligand_1	-1.72	17	7	3	2
Ligand_2	-1.60	18	7	4	2

Table 6 — ADMET analysis of selected drugs

Compounds	GI absorption	BBB permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation)
Ligand_1	High	No	No	No	No	No	No	No	-8.63 cm/s
Ligand_2	High	No	No	No	No	No	No	No	-8.94 cm/s

Table 7 — Physiochemical analysis of selected drugs

Compound	Formula	Molecular weight	Num. heavy atoms	Num. aroma. heavy atoms	Fraction Csp3	Num. rotatable bonds	Num. H-bond acceptors	Num. H-bond donors	Molar Refractivity	TPSA
Ligand_1	$C_9H_{11}FN_2O_5$	246.19 g/mol	17	6	0.56	2	6	3	53.07	104.55 Å²
Ligand_2	$C_9H_{11}F_2N_3O_4$	263.20 g/mol	18	6	0.56	2	7	3	54.83	110.60 Å²

Table.8 — Docking score and interacting residues of selected drugs with FGF2

Compound	Type of bond	Binding affinity (kcal/mol)	Amino acid	Bond length Å
Ligand_1	H-bond	-6.7	His 75	2.47
	Pi alkyl		Ala 83	4.21
	Pi alkyl		Ala 80	4.87
Ligand_2	Pi alkyl	-6.3	Phe 73	3.89

Table.9 — Docking score and interacting residues of selected drugs with ATF3

Compound	Type of bond	Binding affinity (kcal/mol)	Amino acid	Bond length Å
Ligand_1	H-bond	-4.7	Arg150	2.64
Ligand_2	H-bond	-5.0	Arg150	2.89
	Pi alkyl		Lys139	4.40
	Pi alkyl		Phe170	5.23

Table.10 — Docking score and interacting residues of selected drugs with BCL2

Compound	Type of bond	Binding affinity (kcal/mol)	Amino acid	Bond length Å
Ligand_1	H-bond	-5.0	Ser93	2.65
	Pi alkyl		The97	4.98
Ligand_2	H-bond	-5.6	Ser93	2.20
	Pi alkyl		Phe97	3.74

Table 11 — Docking score and interacting residues of selected drugs with HMOX

Compound	Type of bond	Binding affinity (kcal/mol)	Amino acid	Bond length Å
Ligand_1	H bond	-6.7	Asp130	2.95
	Pi alkyl		Ala40	3.42
Ligand_2	H bond	-7.1	Arg126	3.02
	H bond		Asp130	3.21
	Pi alkyl		Val24	4.74
	Pi alkyl		Phe23	5.17

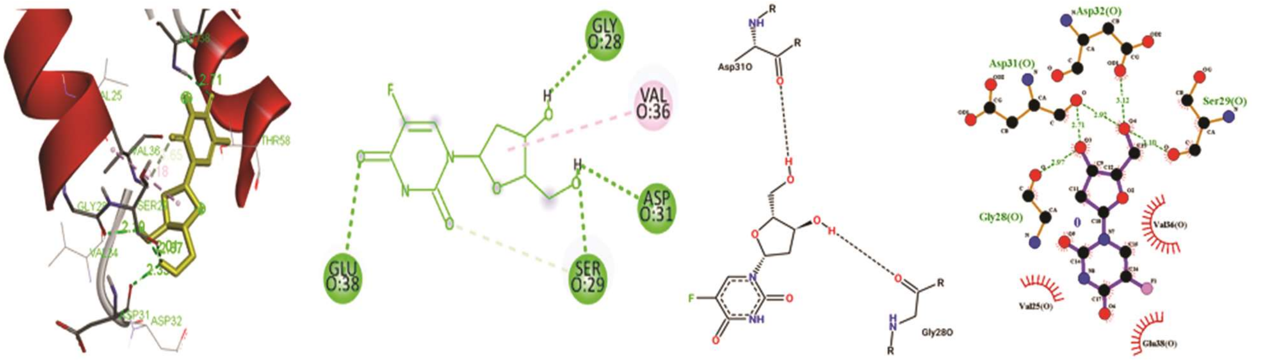


Fig.1 — 2D, 3D and Lig plot docking pose of ID2-ligand complex (a) 5-flurouracil

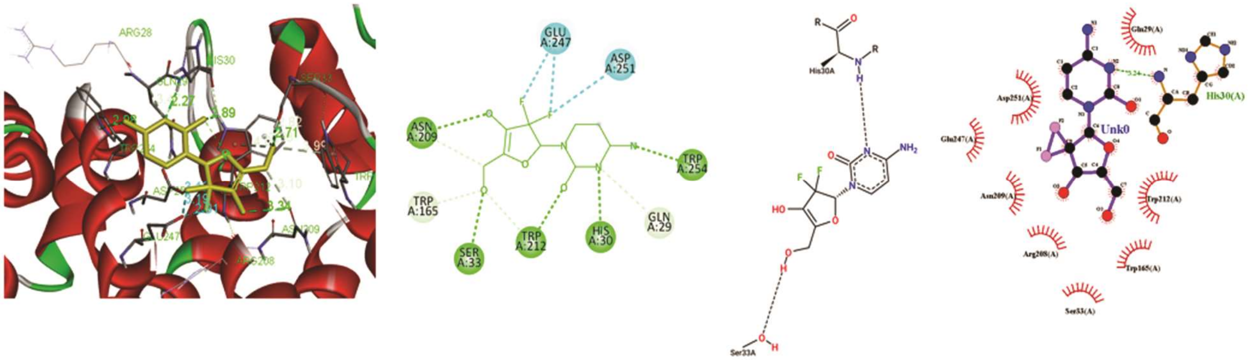


Fig. 2 — 2D, 3D and Lig plot docking pose of CLIC4-ligand complex (a) Gemcitabine

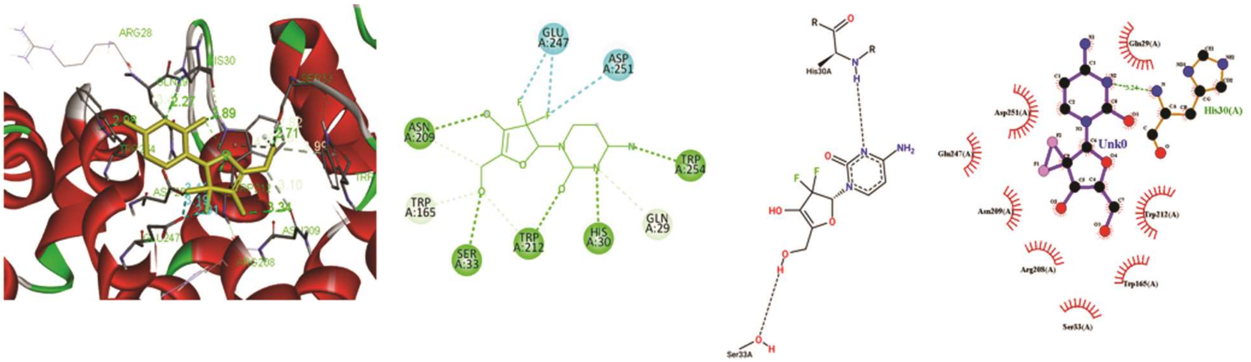


Fig.3 — 2D, 3D and Lig plot docking pose of MED14-ligand complex (a) 5-flurouracil

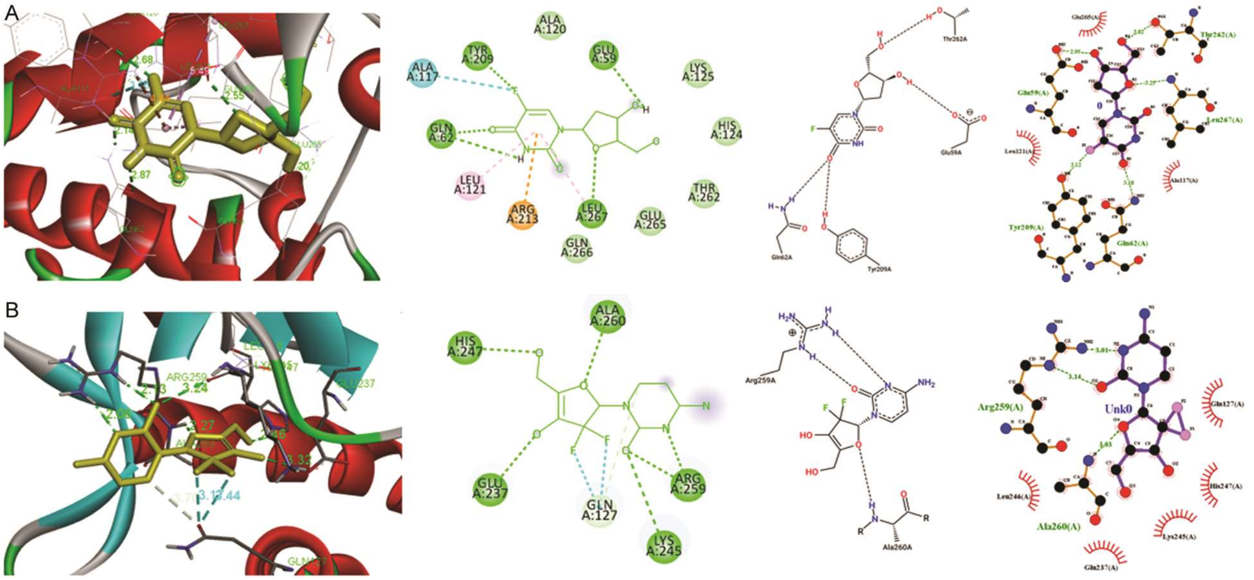


Fig.4 — 2D, 3D and Lig plot docking pose of NGEF-ligand complex (a)5-flurouracil (b) Gemcitabine

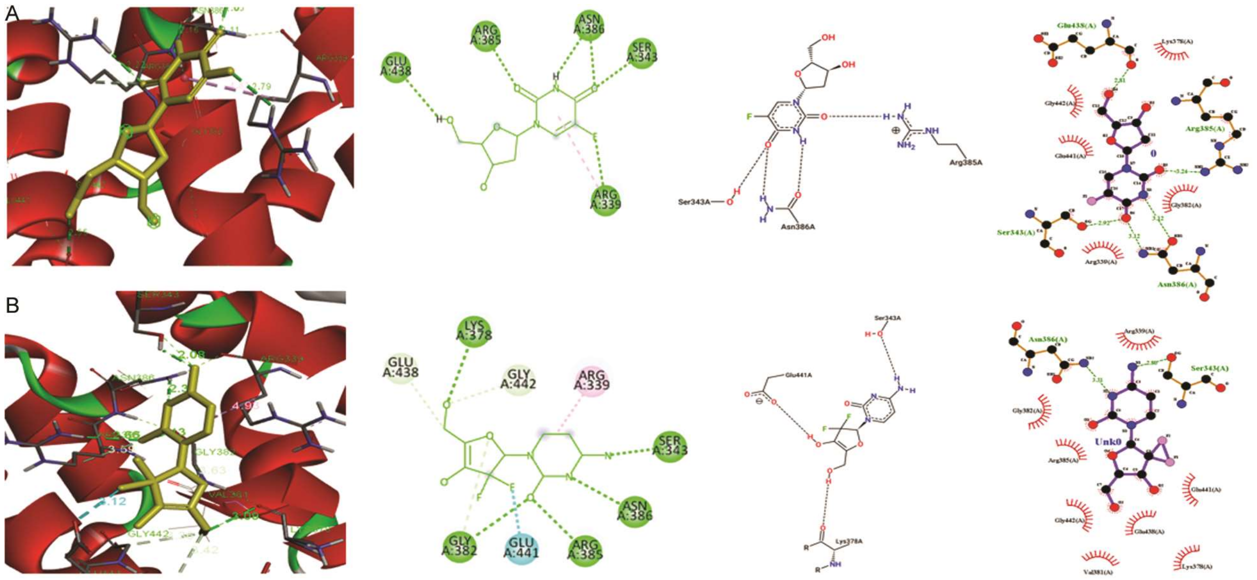


Fig. 5 — 2D, 3D and Lig plot docking pose of TCF4-ligand complex (a) 5-flurouracil (b) Gemcitabine

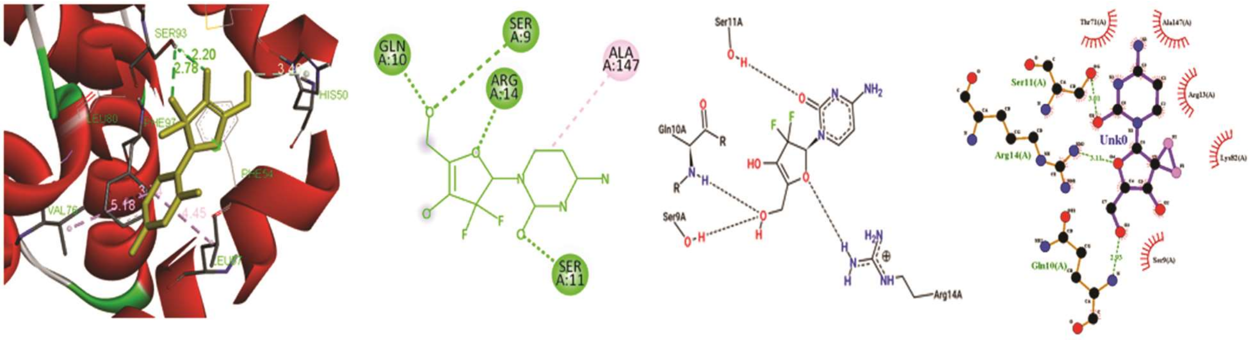


Fig.6 — 2D, 3D and Lig plot docking pose of MAF ligand complex (a) Gemcitabine

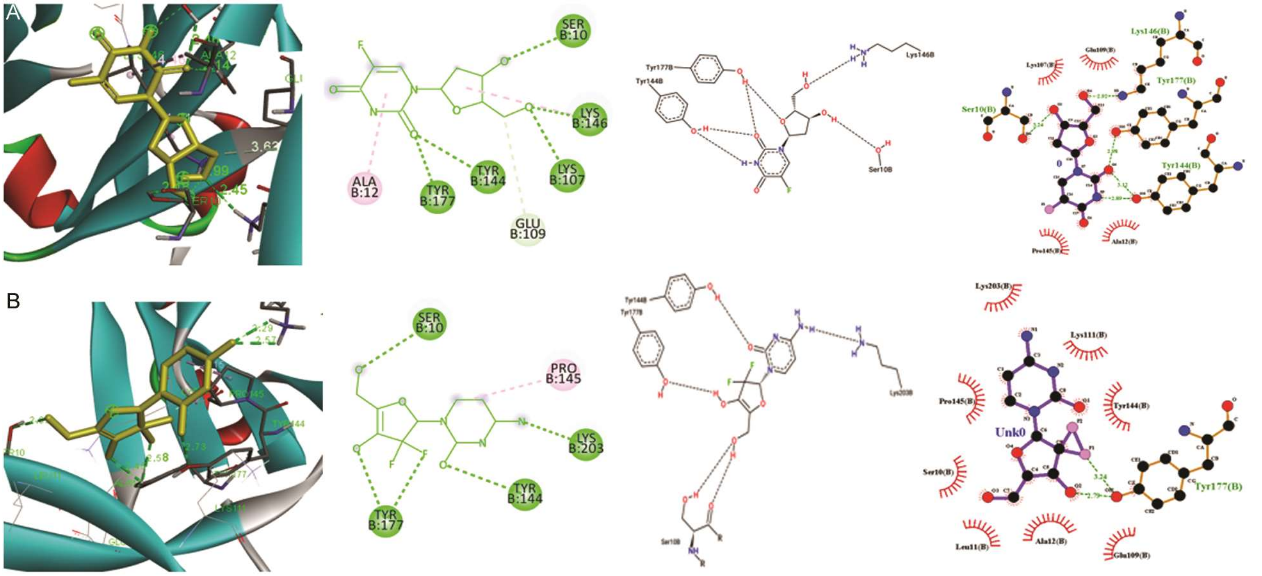


Fig. 7 — 2D, 3D and Lig plot docking pose of MYC -ligand complex (a) 5-flurouracil (b) Gemcitabine

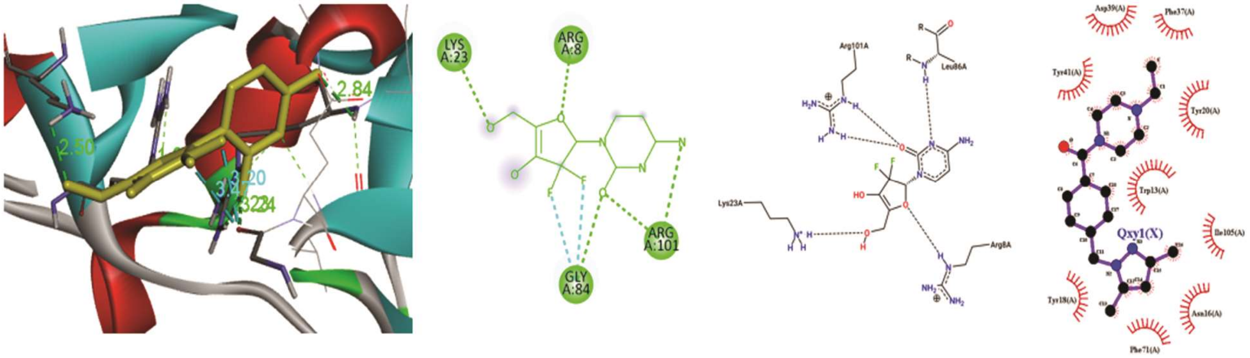
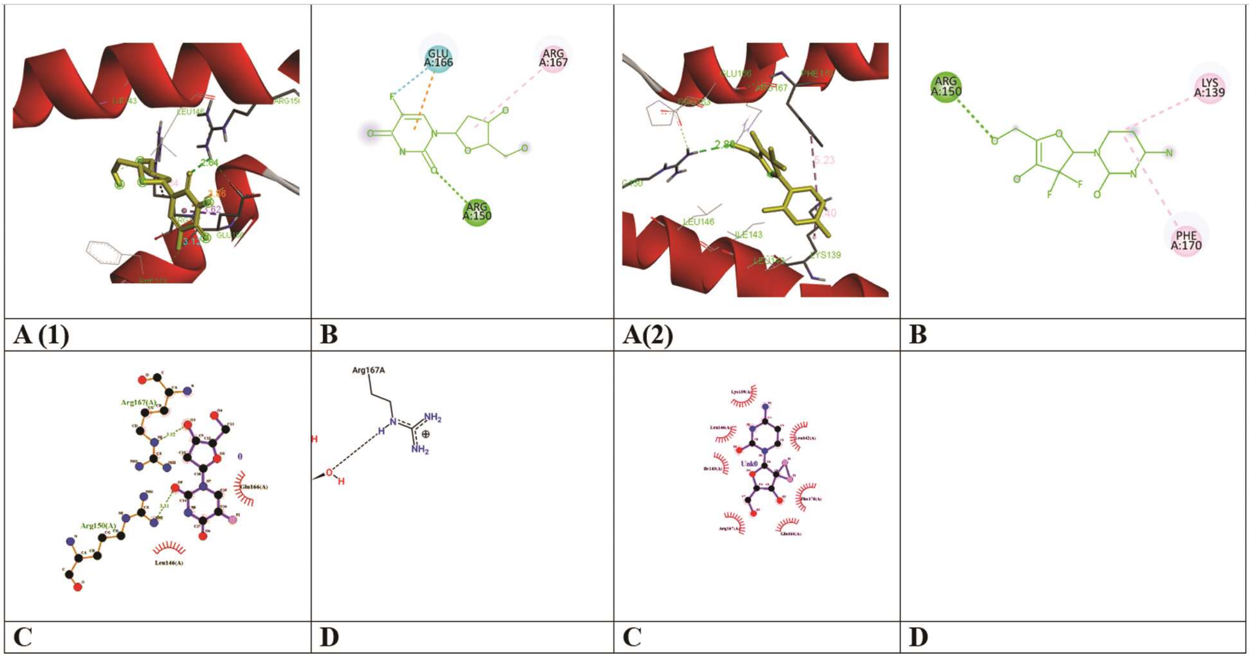
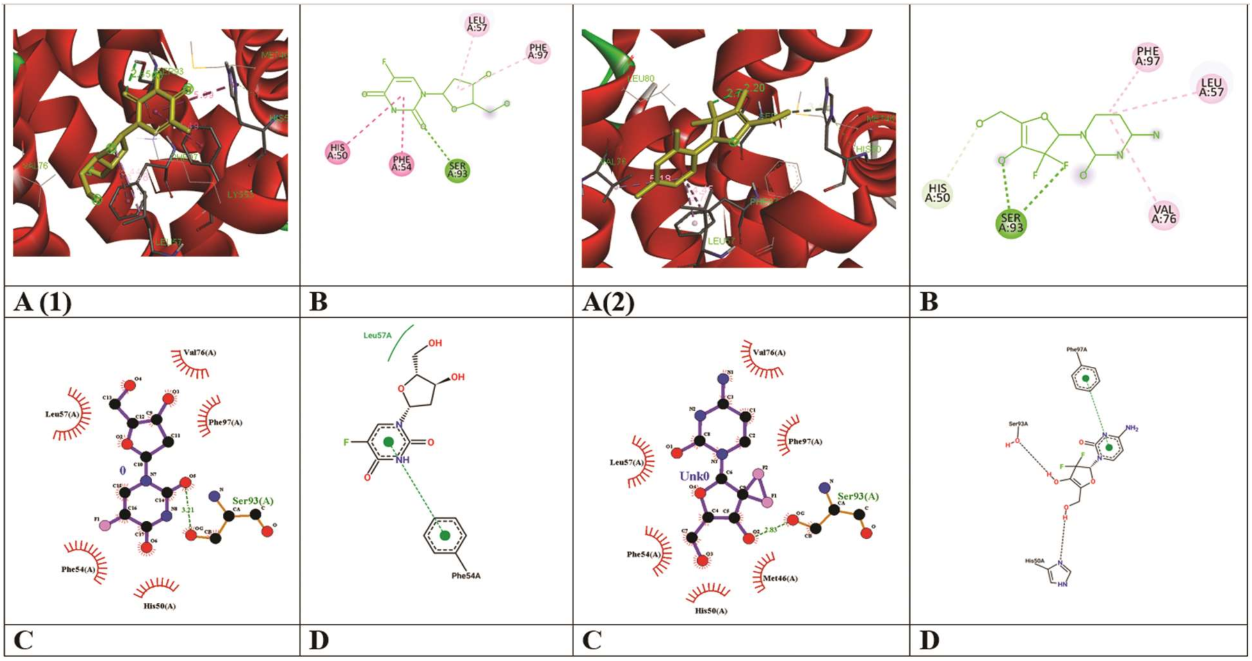
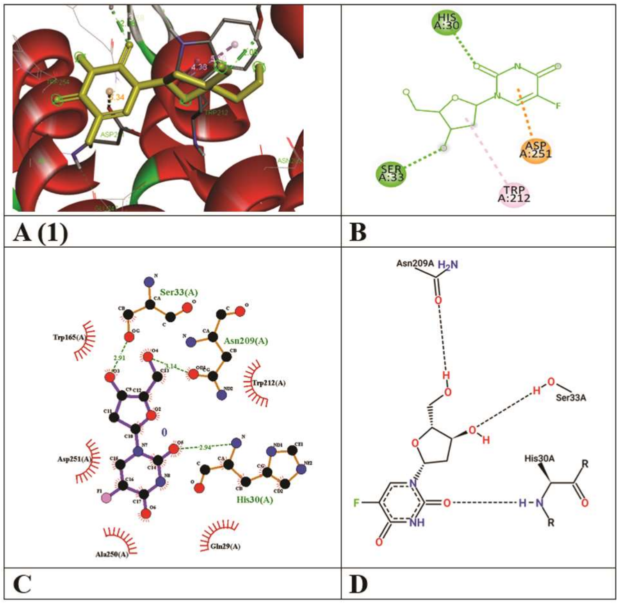
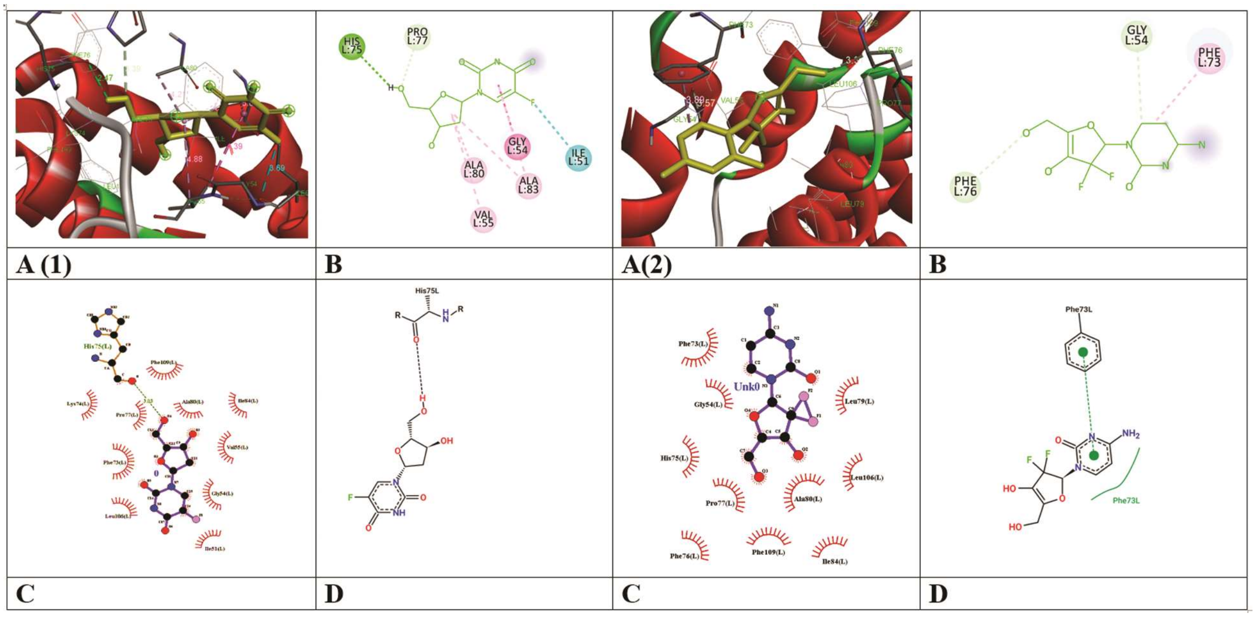


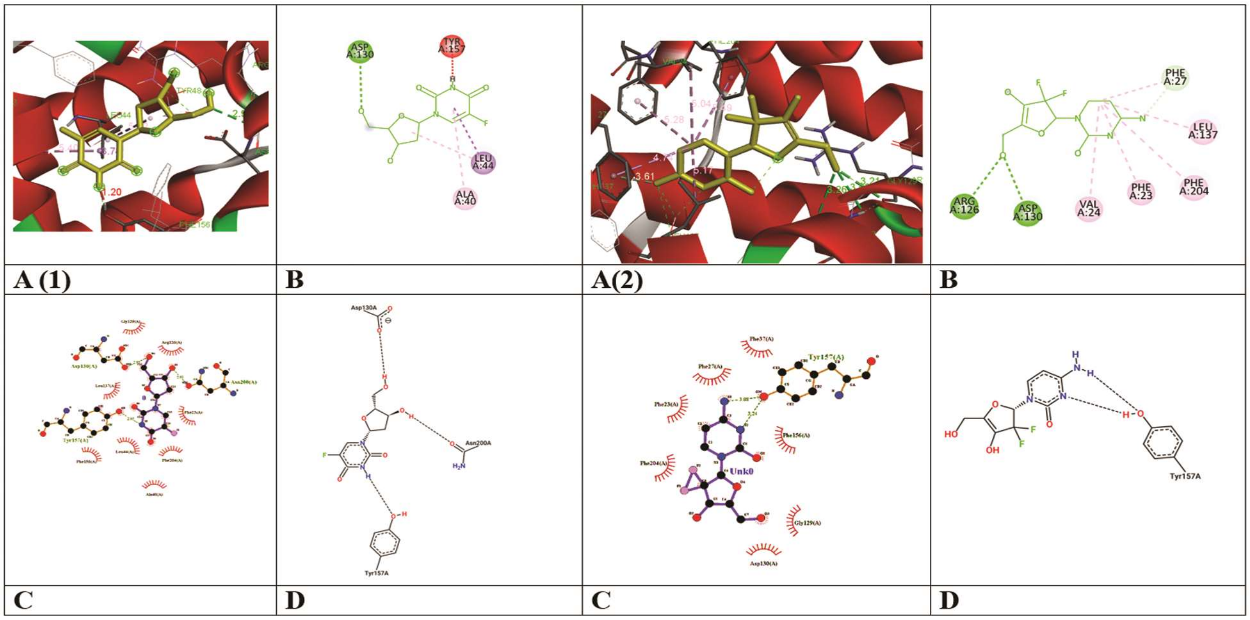
Fig. 8 — 2D, 3D and Lig plot docking pose of TP53 -ligand complex (a) Gemcitabine

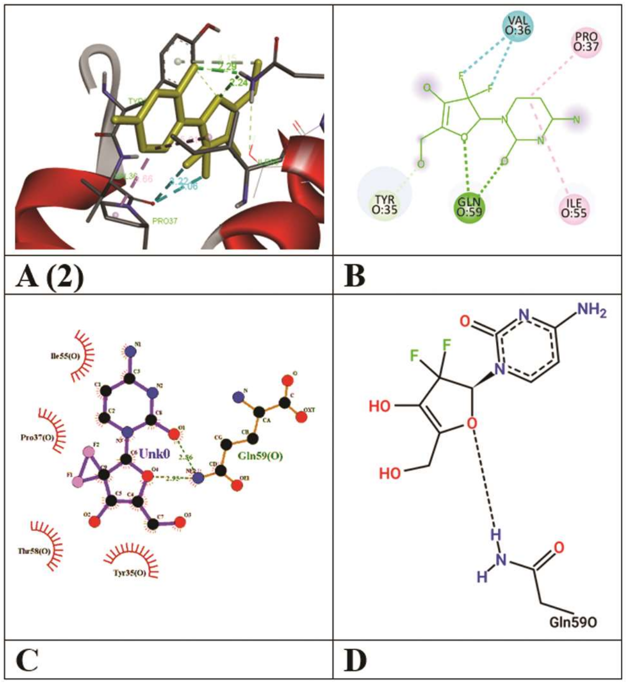

GLU A:166
ARG A:167
ARG A:150
ARG A:150
LYS A:139
PHE A:170
LEU146
ARG150
2.84
GLU166
PHE167
2.88
3.23
LEU146
ILE143
LYS139
A (1)
B
A(2)
B
Arg167(A)
Gln166(A)
Arg150(A)
Leu146(A)
Arg167A
NH2
NH2
Unk0
C
D
C
D

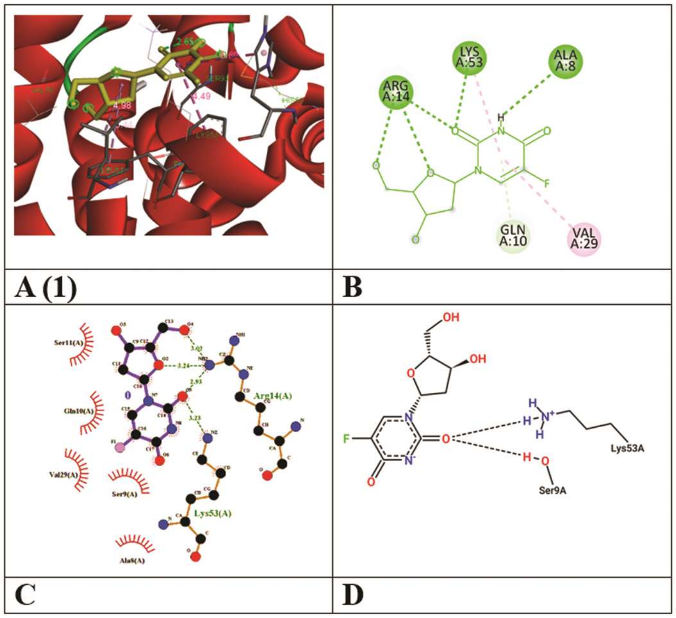

LEU A:57
PHE A:97
HIS A:50
PHE A:54
SER A:93
PHE A:97
LEU A:57
HIS A:50
SER A:93
VAL A:76
LEU80
A (1)
B
A(2)
B
Val76(A)
Leu57(A)
Phe97(A)
Ser93(A)
3.21
Phe54(A)
His50(A)
Leu57A
OH
OH
F
NH
Phe54A
Val76(A)
Phe97(A)
Leu57(A)
Unk0
Ser93(A)
2.83
Phe54(A)
Met46(A)
His50(A)
Phe97A
Ser93A
NH2
His50A
C
D
C
D

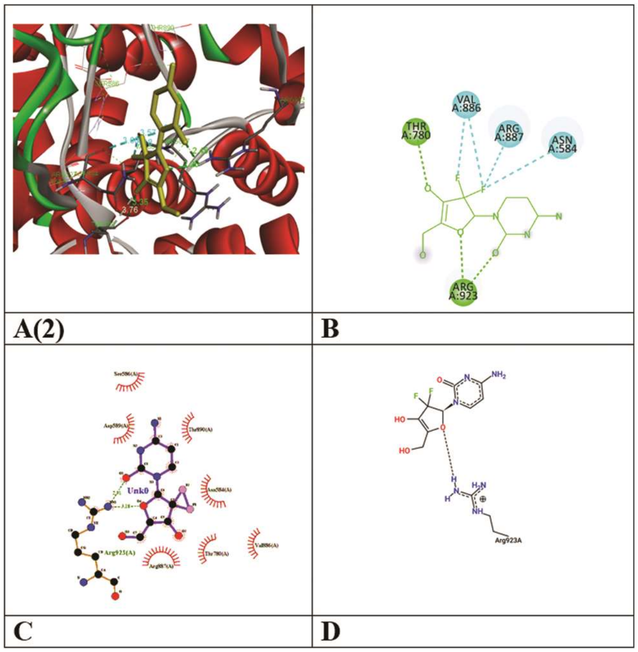

HIS A:30
SER A:33
ASP A:251
TRP A:212
A (1)
B
Ser33(A)
Asn209(A)
Trp165(A)
Trp212(A)
Asp251(A)
His30(A)
Ala250(A)
Gln29(A)
Asn209A
Ser33A
His30A
C
D

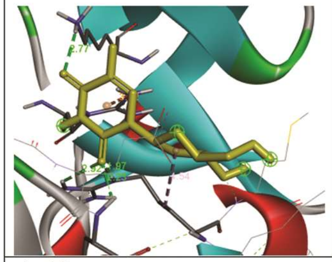

HIS L:75
PRO L:77
GLY L:54
ALA L:80
ALA L:83
ILE L:51
VAL L:55
GLY L:54
PHE L:73
PHE L:76
A (1)
B
A(2)
B
His75(L)
Phe109(L)
Lys74(L)
Pro77(L)
Ala80(L)
Ile84(L)
Val55(L)
Phe75(L)
Gly54(L)
Leu106(L)
Ile51(L)
His75L
Phe73(L)
Unk0
Leu79(L)
Gly54(L)
His75(L)
Leu106(L)
Pro77(L)
Ala80(L)
Phe76(L)
Phe109(L)
Ile84(L)
Phe73L
C
D
C
D


A (1)
B
A(2)
B
C
D
C
D
ASP A:130
TYR A:157
LEU A:44
ALA A:40
PHE A:27
LEU A:137
ARG A:126
ASP A:130
VAL A:24
PHE A:23
PHE A:204
Asp130A
Asn200A
Tyr157A
Tyr157(A)
Phe37(A)
Phe27(A)
Phe23(A)
Phe156(A)
Phe204(A)
Unk0
Gly129(A)
Asp130(A)
Tyr157A

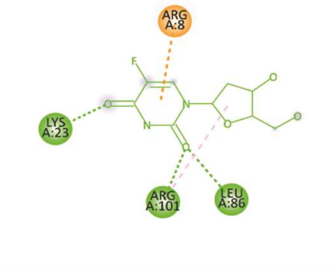

A (2)
B
C
D
PRO37
VAL O:36
PRO O:37
TYR O:35
GLN O:59
ILE O:55
Ile55(O)
Pro37(O)
Unk0
Gln59(O)
2.86
2.95
Thr58(O)
Tyr35(O)
NH2
HO
HO
F
F
O
N
Gln59O


A (1)
B
C
D
ARG A:14
LYS A:53
ALA A:8
GLN A:10
VAL A:29
Ser11(A)
Gln10(A)
Val29(A)
Ser9(A)
Arg14(A)
Lys53(A)
Ala8(A)
3.02
3.24
2.93
3.23
OH
F
O
Lys53A
Ser9A

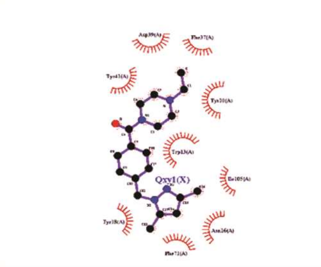

A(2)
B
C
D
THR A:780
VAL A:886
ARG A:887
ASN A:584
ARG A:923
3.76
Ser586(A)
Asp589(A)
Thr890(A)
Asn584(A)
Unk0
Arg923(A)
Arg887(A)
Thr780(A)
Val886(A)
HO
F
NH_2
Arg923A


2.77
2.92
2.97

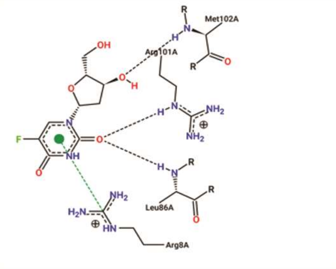
A (1)


ARG A:8
F
LYS A:23
N
ARG A:101
LEU A:86

B


Arg109(A)
Phe37(A)
Tyr43(A)
Tyr101(A)
Trp13(A)
Qxv1(X)
Ile105(A)
Tyr18(A)
Asn26(A)
Phe72(A)

C


Met102A
Arg101A
OH
H
NH2
F
NH
H2N
Leu86A
Arg8A

D