

### Supplementary data

#### Synthesis, in-silico screening and preclinical evaluation studies of hexapeptide analogue for its antimicrobial efficacy

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**Table S1- Interaction residues of control ligands with pdb**

Control ligands	H bond	Salt bridges	Pi cation	Bond length with Lys 274
cephalexin	Lys 274, val 354, Tyr 315, Gln 271, Glu 233	Arg 325	Lys 274	1.79, 3.91
cefotaxime	Glu 290, Arg 286, Arg 286, Lys 274, Asn 275, Gly 259	Lys 274		3.85, 2.75
vancomycin	Leu 278, Leu 278, Asn 275, Glu 211, Glu 211, Glu 323, Glu 281, Gly 259, Lys 274	Lys 274	Arg 286, Arg 325	1.98
ciprofloxacin	Asn 275, Val 354,	Glu 323	Arg 325	
menomycin	Leu 278, Ser 279, Lys 355, Gln 271, Try 315, Lys 274, Lys 274, Gly 259, Tyr 360, Arg 286, Glu 281, Glu 211, Asn 275, Arg 325			1.89,1.79
AMP	Glu 323, Glu 323, Glu 281, Lys 274, Lys 274, Ser 358, Ser 358, Arg 364, Thr 257, Glu 233			1.94, 2.79

**Table S2- Interactive score with different control**

ligand	GScore	DockScore	LipophilicEvdW	HBond	Electro	HBond	Electro
3VMAppwduplicate_molecule1	-14.24	-14.24	-2.03	-10.23	-2	-10.23	-2
sequence_pep.mol	-9.22	-9.22	-3.04	-3.7	-3.3	-3.7	-3.3
ciprofloxacin	-4.55	-3.25	-1.18	-2.4	-0.95	-2.4	-0.95
Vancomycin1.mol-2	-8	-6.81	-2.78	-3.75	-2	-3.75	-2
Cefotaxime1.mol	-5.17	-5.17	-1.49	-2.67	-1.3	-2.67	-1.3
Cephalexin1.mol	-4.4	-4.34	-0.91	-1.83	-2.31	-1.83	-2.31

Fig F1- 2D and 3D interaction diagram with cefotaxime

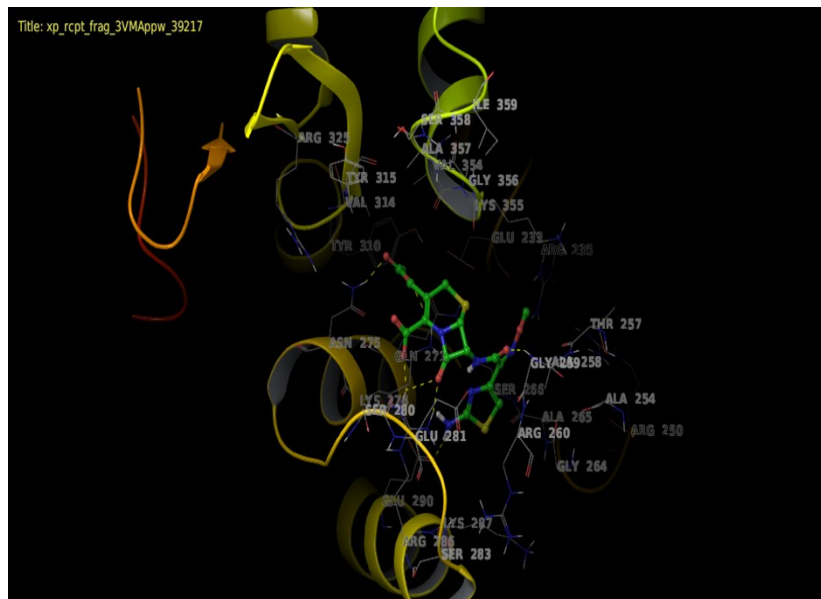
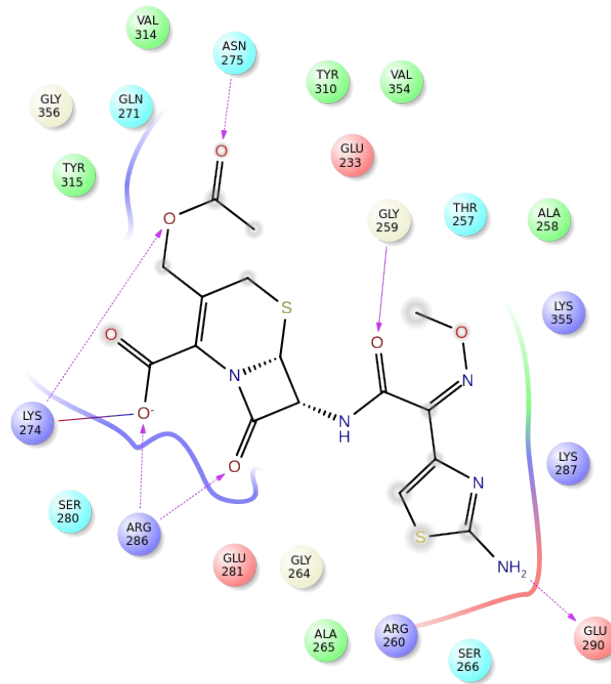


Fig F2- 2D and 3D interaction diagram with cephalixin

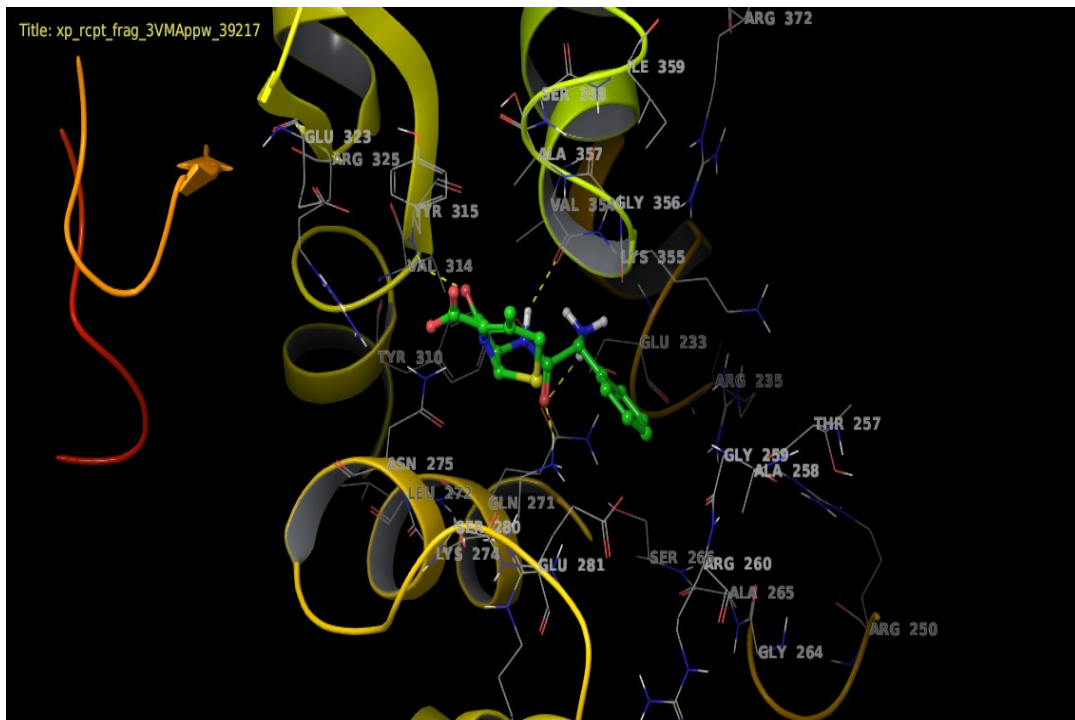
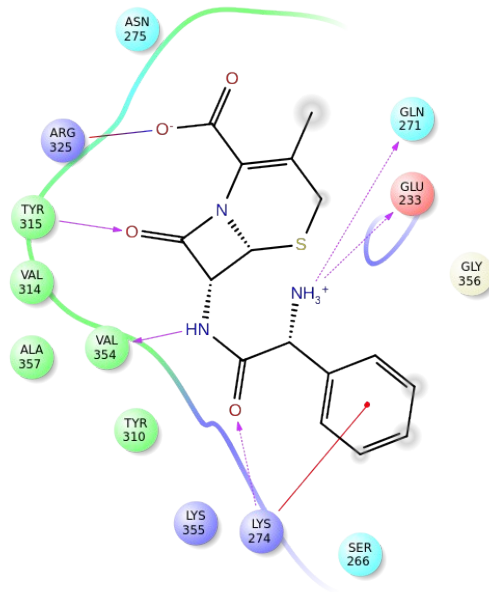
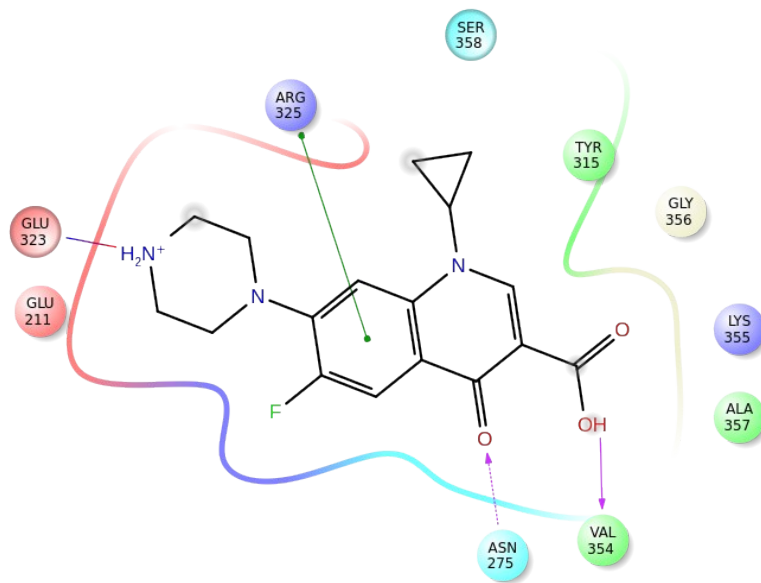


Fig F3- 2D and 3D interaction diagram with ciprofloxacin



Title: xp\_rcpt\_frag\_3VMAppw\_3060

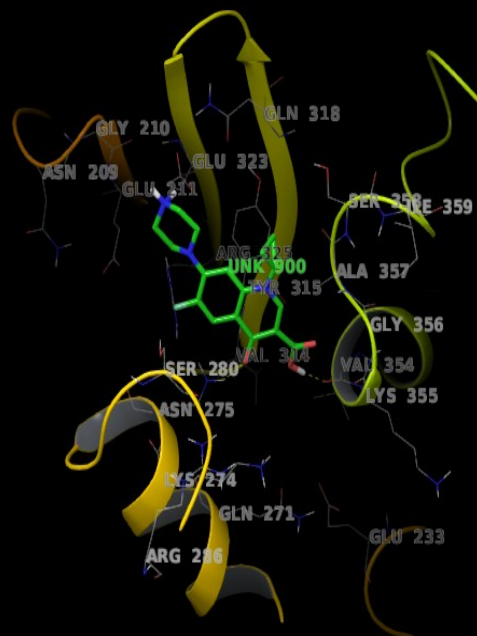


Fig F4- 2D and 3D interaction diagram with vancomycin

