BIOINFORMATION

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Supplementary material:

Table 1: Mutations at catalytic triad of NS2B-NS3 complex

NS2B-NS3 complex	HIS 94	ASP 118	SER 176
NS2B-NS3 Δ_1	*ALA*	*ALA*	*ALA*
NS2B-NS3 Δ_2	*ALA*	*ALA*	*CYS*
NS2B-NS3 Δ_3	*ALA*	*ASN*	*ALA*
NS2B-NS3 Δ_4	*ALA*	*ASN*	*CYS*

Table 2: Hydrogen bonds formed before mutation

H-bond	Residue 1(B1)	Atom	Residue 2 (B2)	Atom	B1-B2 distance (Å)
1	94 HIS	N	118 ASP	OD1	3.27
2	94 HIS	N	118 ASP	OD2	3.28
3	118 ASP	N	115 VAL	O	3.02
4	118 ASP	N	114 SER	O	2.70
5	179 SER	N	176 SER	O	3.19

Table 3a: Hydrogen bonds formed after mutation

H-bonds	Residue 1 (B1)	Atom	Residue 2 (B2)	Atom	B1-B2 distance (Å)
1	118 ASP	N	115 VAL	O	3.02
2	118 ASP	N	114 SER	O	2.70
3	179 SER	N	176 SER	O	3.19

Table 3b: RMSD values of the mutated models

Mutants	RMSD(Å)
NS2B-NS3 Δ_1	15.952
NS2B-NS3 Δ_2	4.706
NS2B-NS3 Δ_3	4.798
NS2B-NS3 Δ_4	7.929

Table 4: Docking of the ligands (4-hydroxypanduratin A, Panduratin A and Ester) with NS2B-NS3 complex

Ligand	Binding Energy (kcal/mol)	Number of Hydrogen bonds	Inhibitory Constant (μM)	Interacting with catalytic triad (His 94, Asp 118, Ser 176)
4-hydroxypanduratin A	-5.44	2	103.73	Yes
Panduratin A	-5.76	2	60.26	No
Ester	-4.27	4	740.49	No