

Supporting Information

Paritaprevir as a Pan-antiviral Against Different Flaviviruses

R.P. Yadav^a and N.R. Jena^{a*}

^aDiscipline of Natural Sciences, Indian Institute of Information Technology, Design and Manufacturing, Dumna Airport Road, Jabalpur-482005, India

Corresponding Author's Email Address: nrjena@iiitdmj.ac.in

Table S1: The MM/PBSA binding free energies (ΔG_{bind}) of different complexes and contributions of different energies to the ΔG_{bind} . All energies are provided in kcal/mol.

Sl No	Complexes	ΔG_{bind}	ΔE_{vdw}	ΔE_{Elec}	ΔE_{PB}	ΔE_{NP}	ΔE_{Disp}
1	ZIKV-Ritonavir	-17.4 $\pm$ 3.18	-44.2 $\pm$ 3.23	-7.43 $\pm$ 2.89	11.52 $\pm$ 2.8	-30.55 $\pm$ 2.05	53.2 $\pm$ 2.41
2	ZIKV-Saquinavir	-5.03 $\pm$ 2.90	-34.7 $\pm$ 3.23	-0.57 $\pm$ 1.65	7.48 $\pm$ 1.61	-22.11 $\pm$ 1.93	46.8 $\pm$ 2.52
3	ZIKV-Indinavir	-2.95 $\pm$ 3.55	-15.4 $\pm$ 5.9	-2.03 $\pm$ 2.19	3.79 $\pm$ 1.8	-12.06 $\pm$ 4.86	22.82 $\pm$ 7.40
4	ZIKV-Paritaprevir	-14.2 $\pm$ 3.14	-48.8 $\pm$ 2.84	-7.16 $\pm$ 1.20	13.2 $\pm$ 1.30	-29.94 $\pm$ 1.36	58.45 $\pm$ 1.96
5	ZIKV-Lopinavir	-7.33 $\pm$ 2.56	-30.8 $\pm$ 3.03	-7.3 $\pm$ 1.26	9.72 $\pm$ 1.34	-22.40 $\pm$ 2.13	43.54 $\pm$ 2.76
6	WNV-Ritonavir	-7.43 $\pm$ 2.16	-30.64 $\pm$ 1.92	-2.07 $\pm$ 0.58	6.58 $\pm$ 0.57	-22.0 $\pm$ 1.15	40.79 $\pm$ 1.29
7	WNV-Paritaprevir	-17.3 $\pm$ 2.55	-51.5 $\pm$ 2.75	-6.74 $\pm$ 1.11	12.40 $\pm$ 1.19	-33.4 $\pm$ 1.39	61.9 $\pm$ 2.05
8	DENV-Ritonavir	-11.5 $\pm$ 2.82	-39.32 $\pm$ 3.25	-5.24 $\pm$ 1.28	9.08 $\pm$ 1.40	-27.6 $\pm$ 2.30	51.6 $\pm$ 3.00
9	DENV-Paritaprevir	-12.7 $\pm$ 2.91	-51.7 $\pm$ 3.88	-4.29 $\pm$ 1.04	11.7 $\pm$ 1.53	-32.08 $\pm$ 2.17	63.6 $\pm$ 3.34

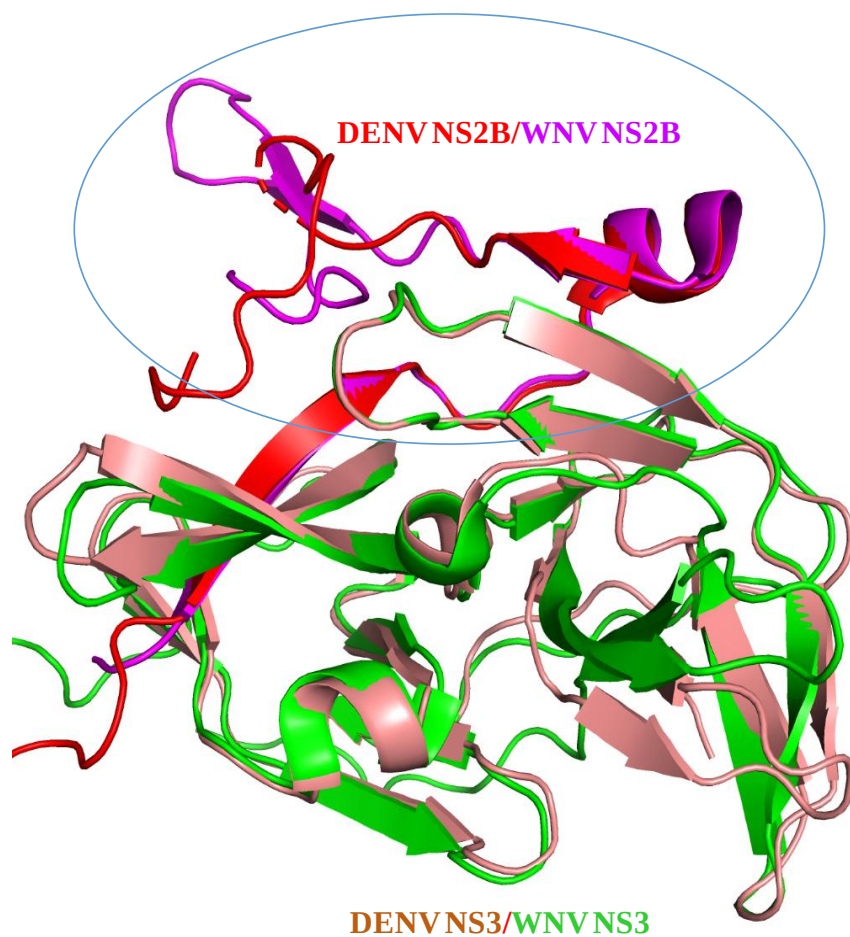


Fig. S1: Comparison of N2B (marked in a circle) and NS3 proteins of the WNV and DENV Proteases.

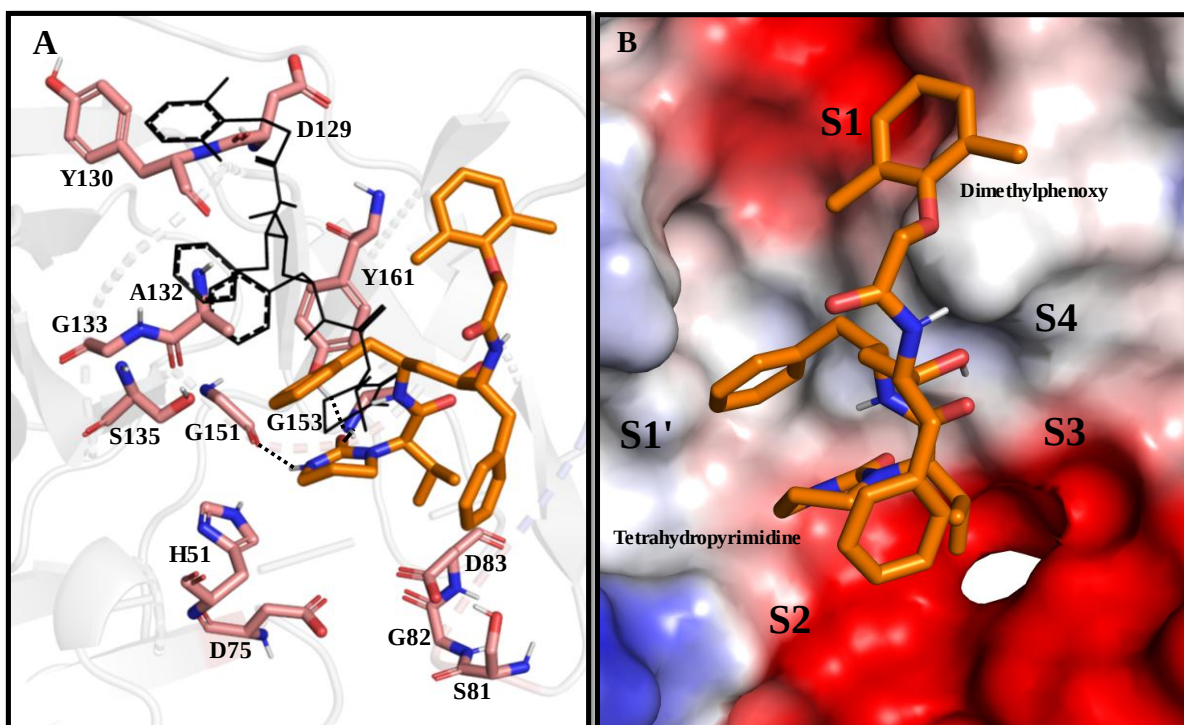


Fig. S2: Average MD-structure of ZIKV protease-Lopinavir complex. (A) Interaction of Lopinavir with different residues of the ZIKV protease and (B) Placement of Lopinavir in the electrostatic surface of the protease.

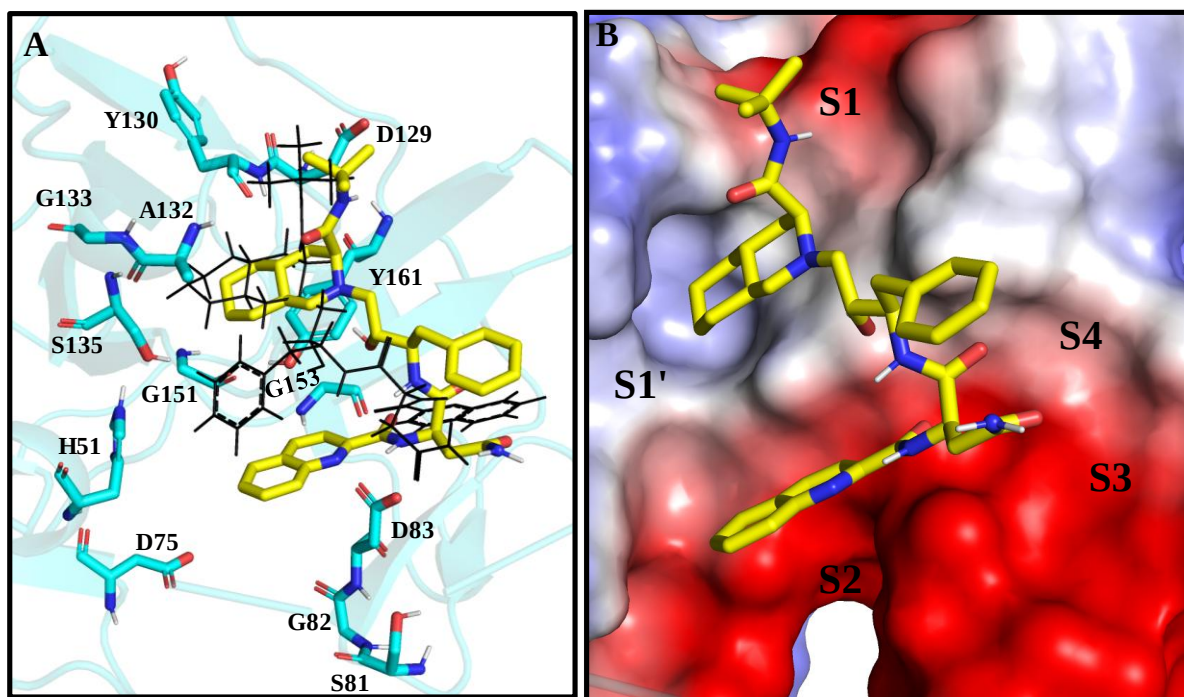


Fig. S3: Average MD-structure of ZIKV protease-Saquinavir complex. (A) Interaction of Saquinavir with different residues of the ZIKV protease and (B) Placement of Saquinavir in the electrostatic surface of the protease.

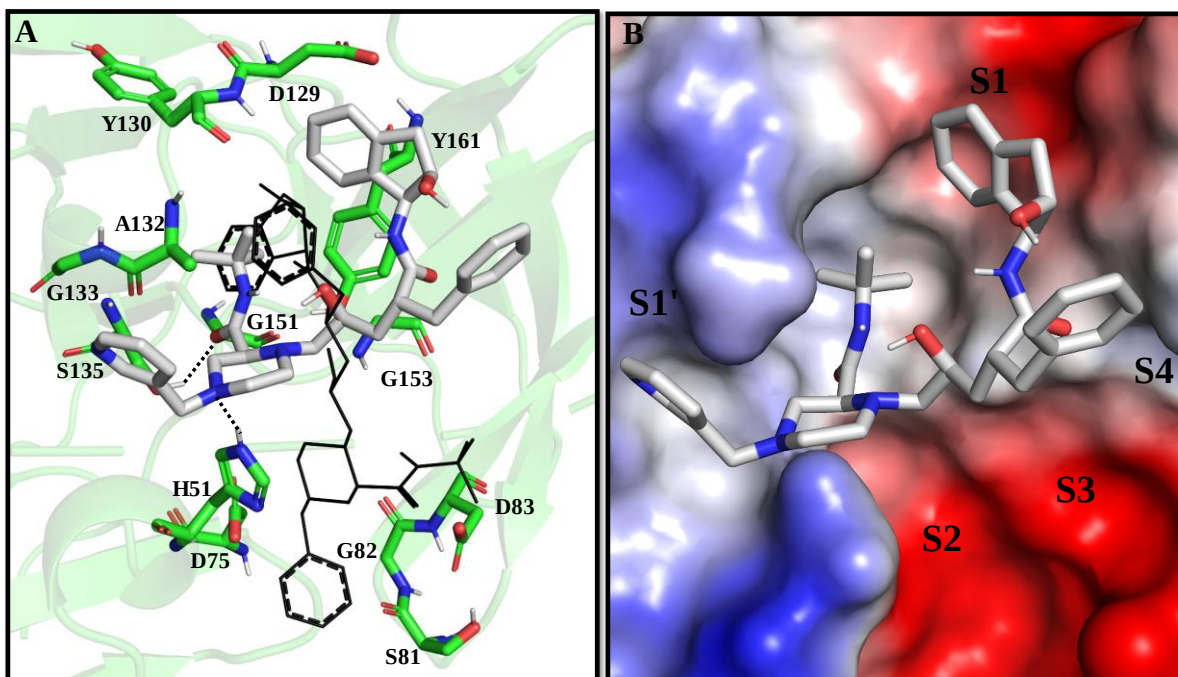


Fig. S4: Average MD-structure of ZIKV protease-Indinavir complex. (A) Interaction of Indinavir with different residues of the ZIKV protease and (B) Placement of Indinavir in the electrostatic surface of the protease.

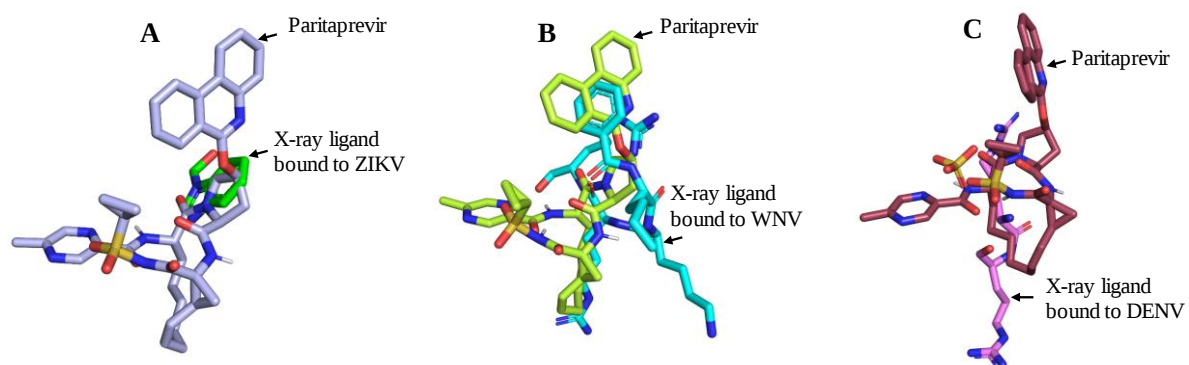


Fig. S5: Comparison of binding modes of Paritaprevir with those of different ligands bound to (A) ZIKV (PDB ID 5H4I), (B) WNV (PDB ID 2PF7), and (C) DENV (PDB ID 3UI1).