# SUPPLEMENTARY INFORMATION

## Role of Disulfide Bonds in Membrane Partitioning of a Viral Peptide

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| Systems | System size | Simulation time (ns) | $n_w$ |
|---|---|---|---|
| SS11-47 – POPC | 101395 | 500 | 69 |
| SS11-52 – POPC | 105965 | 530 | 74 |
| SS47-52 – POPC | 105941 | 580 | 74 |

**Table S1** Details of systems considered in the present study. All atom MD simulations of HAV-2B peptide in three possible disulfide (SS) bonded states are performed in POPC bilayer. The system size denoted by total number of atoms; followed by the simulation time and the number of hydrating water molecules / lipid, $n_w$ are provided as well.

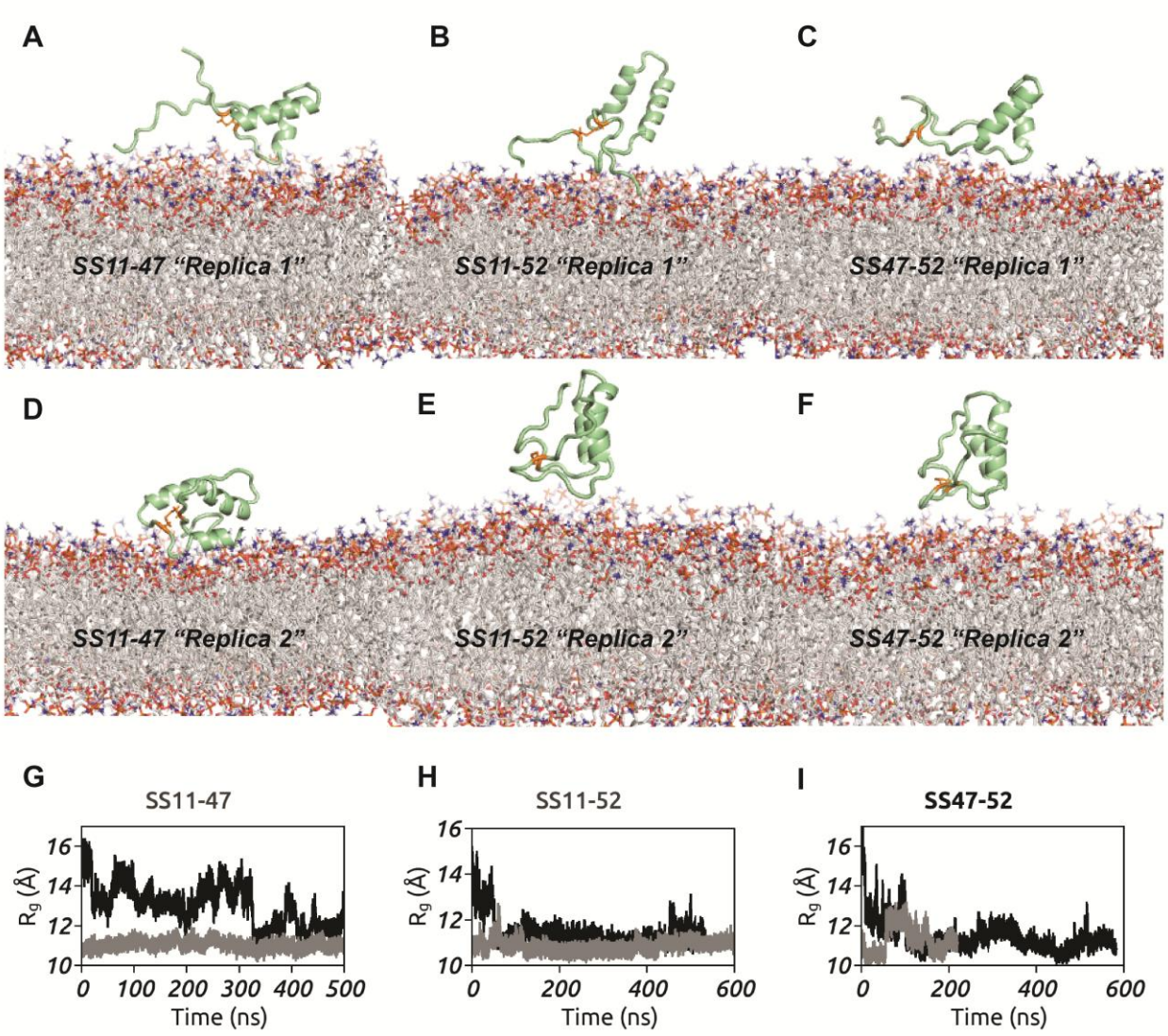


**Fig. S1** The initial peptide-membrane system setups for the three SS-linked states corresponding to two sets of simulations considering different peptide conformations and orientations on POPC bilayer are shown (a-f). The time evolution of radius of gyration, $R_g$, from the two sets of simulations (*Replica 1* in black and *Replica 2* in gray) corresponding to the three SS-linked states indicating disulfide bond induced compact conformation of HAV-2B peptide irrespective of differences in initial peptide conformation.

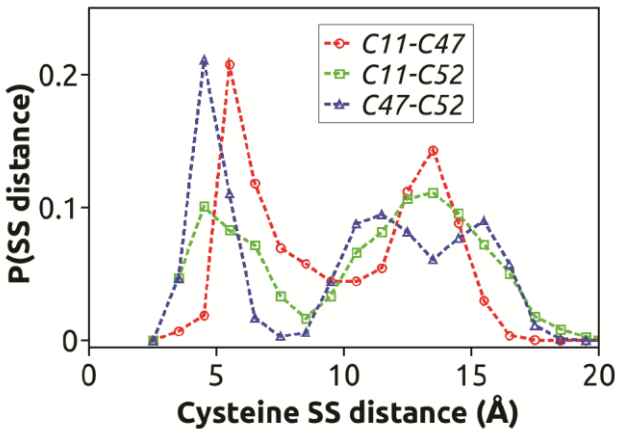


**Fig. S2** Distribution of inter-Cysteine distances calculated considering the thiol "S" atom, from SS-free HAV-2B peptide in water simulation trajectory.

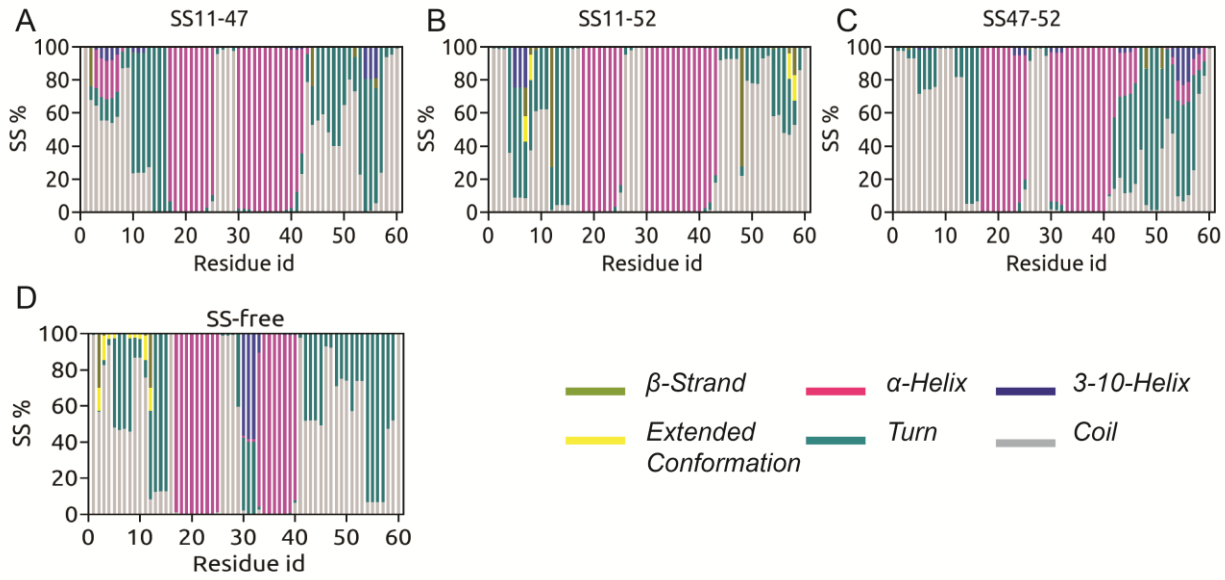


**Fig. S3** Residue based secondary structure percentage % of (A) SS11-47, (B) SS11-52, (C) SS47-52 and (D) SS-free HAV-2B peptide showing population of different secondary structural elements accessible to each residue.

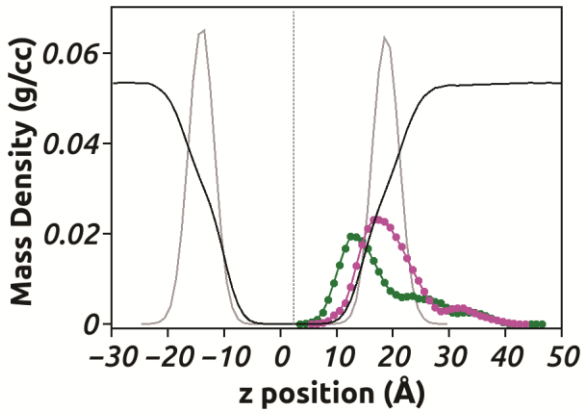


**Fig. S4** The mass density profiles along the bilayer normal (z-direction) of SS-free HAV-2B peptide in POPC bilayer. The density profiles comprising of hydrophobic (green) and hydrophilic (magenta) residues of peptide, phosphate headgroups (grey) and water (reduced by factor of 10, black) are indicated.