Supplementary Figures S1-S2

for

Computational prediction of cyclotides from *Viola odorata* as potential inhibitors against the neuraminidase of *Streptococcus pneumoniae*

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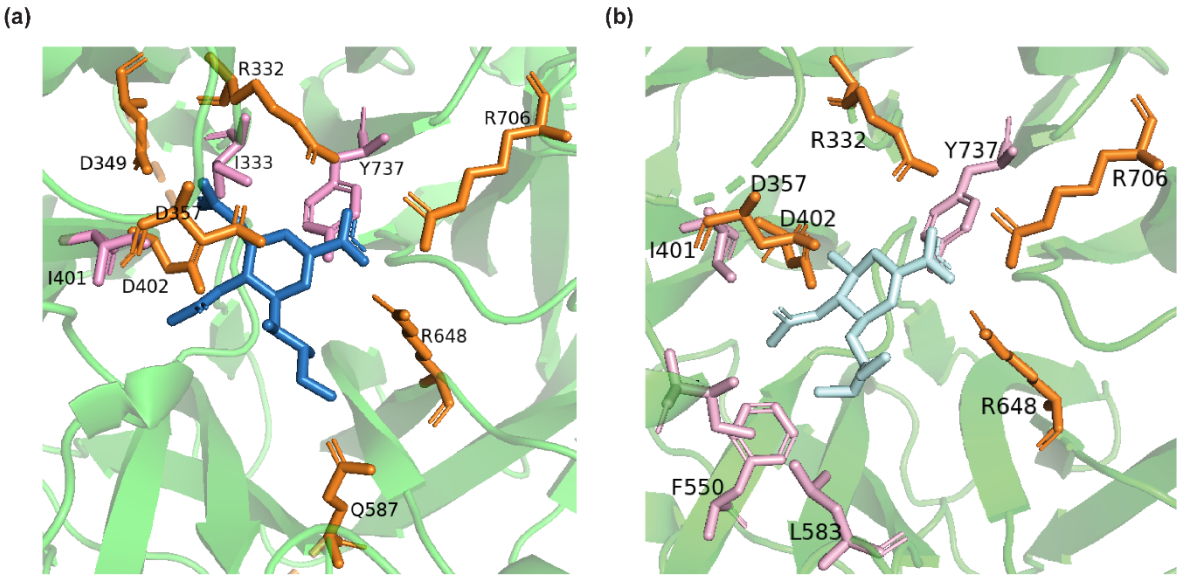

Figure S1: Cartoon representation of non-covalent interaction of the protein *Sp*NanA with the two small molecule reference inhibitors namely, zanamivir and oseltamivir carboxylate in the co-crystallized protein-ligand complex. In each case, the amino acid residues shown in orange sticks represent hydrogen bond interactions with the inhibitor, and the amino acid residues shown in magenta sticks represent hydrophobic interactions with the inhibitor. The atoms in the inhibitors are shown in blue for **(a)** zanamivir and cyan for **(b)** oseltamivir carboxylate.

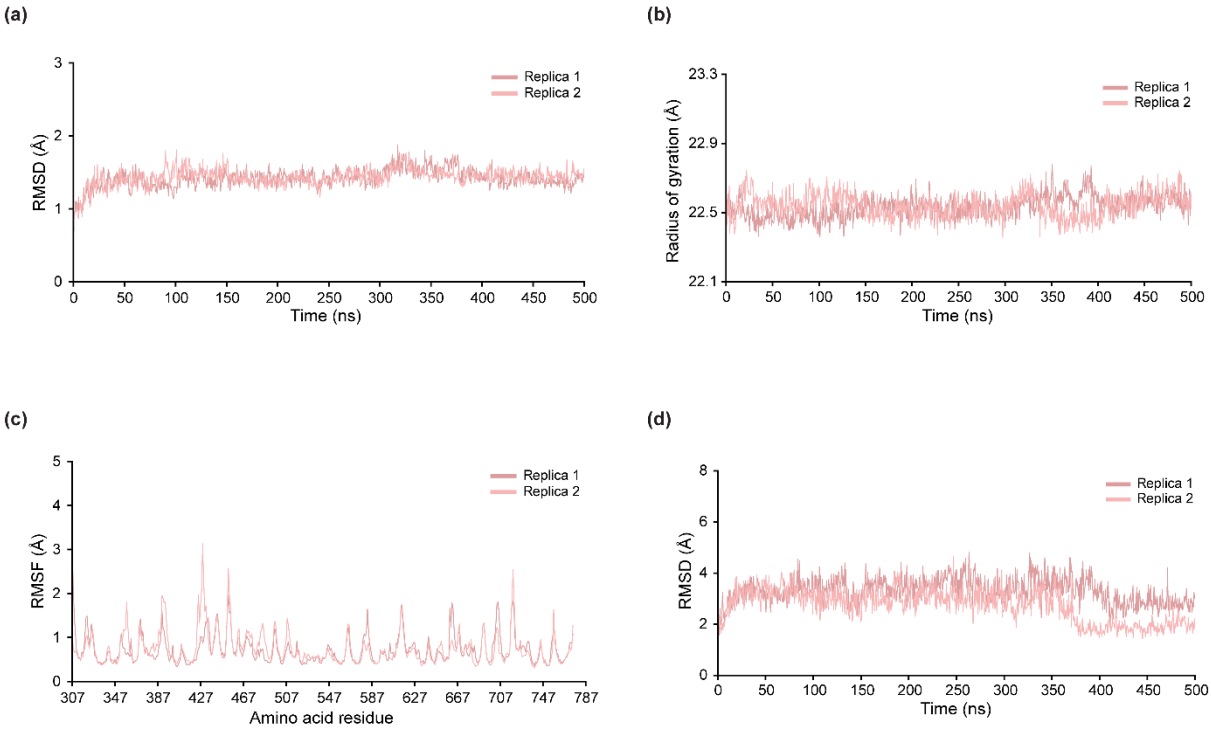

Figure S2: Analysis of MD trajectories from 500 ns simulation (in duplicate; replica 1 and replica 2) of the co-crystallized protein-ligand complex for the small molecule inhibitor, zanamivir. **(a)** RMSD of the Cα atoms of amino acid residues in *Sp*NanA within the protein-ligand complex. **(b)** Radius of gyration **(**R_g) of the *Sp*NanA protein structure within the protein-ligand complex. **(c)** RMSF of the Cα atoms of amino acid residues in *Sp*NanA within the protein-ligand complex. **(d)** RMSD of the heavy (non-hydrogen) atoms of the ligand within the protein-ligand complex.