Results

HVGGSSV binds to the PDZ domain of TIP1

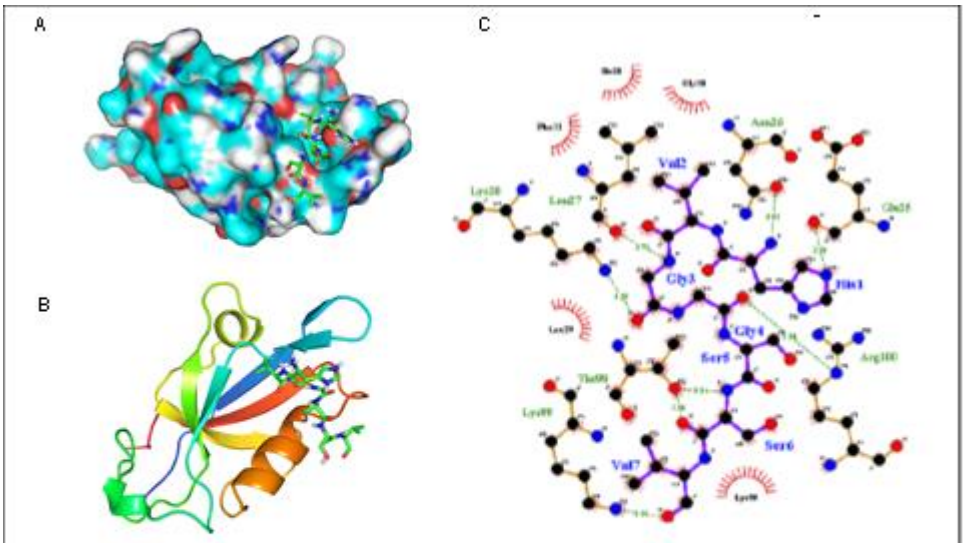

Figure 1. Docking of HVGGSSV peptide into TIP1. (A) HVGGSSV (shown in stick representation) binding in the deep pocket on the TIP1 protein surface. (B) Cartoon representation of TIP1, showing binding of HVGGSSV (stick representation) between the α-helix and anti-parallel β-sheet. (C)Two- dimensional representation of interaction observed between TIP1 and HVGGSSV. Hydrogen bonds are identified by dashed lines, and hydrophobic interactions are shown as arcs. The figure was made by using LIGPLOT program.

Energy-minimized TIP1 protein was docked with energy-minimized HVGGSSV peptide using Autodock Vina software [17]. The binding energy of HVGGSSV to TIP1 calculated by the software was -6.0 kCal/mol. We compared the binding energy of HVGGSSV to other potential peptides. We performed computational docking for the peptide sequences of iCAL36 (ANSRWPTSII), Kir2.3 (RRESI) and Glutaminase L (KENLESMV). The binding energies of these peptides to TIP1 were -6.1, -5.9 and -4.9 respectively **(Supplementary table)**. **Fig 1A** shows HVGGSSV perfectly fitting in the major groove of the TIP1 protein surface. **Fig 1B** shows the peptide fits between the alpha helix and the anti-parallel beta sheets. **Fig 1C** shows the detailed interactions between the amino acids of the protein and the peptide. The TIP1 residues involved in interacting with HVGGSSV are Lys 20, Glu 25, Asn 26, Leu 27, Ile 28, Leu 29,

Supplementary Table. Binding energies of TIP1 binding peptides using computational docking

TIP1 binding ligand	Ligand peptide sequence	Binding energy (kCal/mol)
iCal	ANSRWPTSII	-6.1
Glutaminase L	KENLESMV	-4.9
Kir2.3	RRESI	-5.9