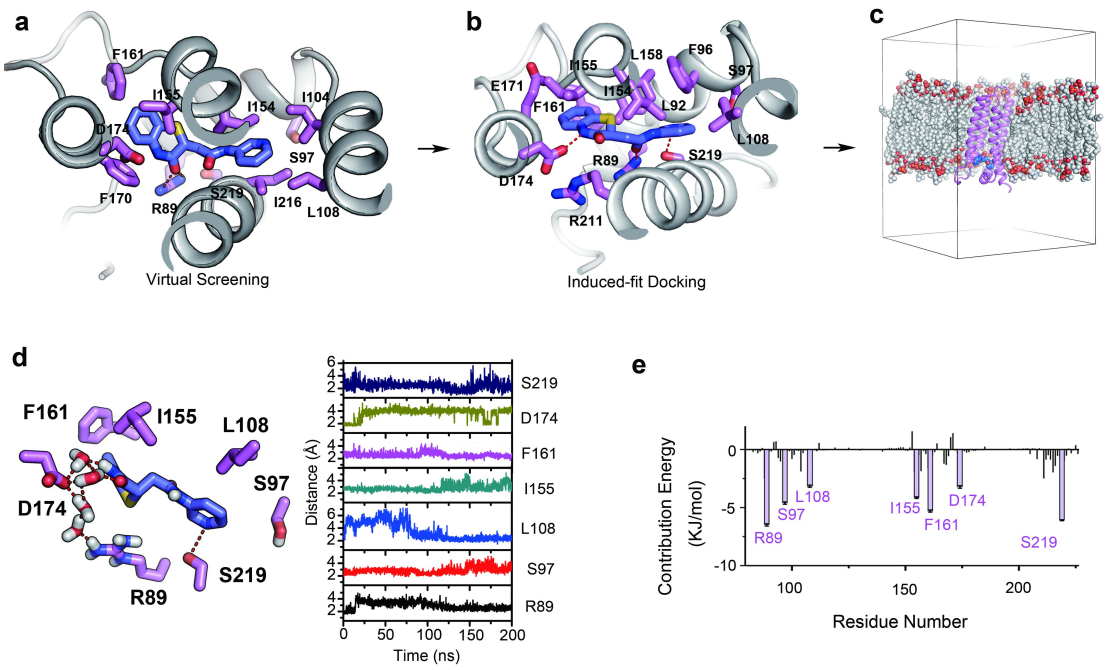

Fig. S5. Binding models of YHV98-1 in Hv1 channel suggested by docking and MD simulation. a Binding mode of YHV98-1 yielded by SP docking of the virtual screening. **b** Binding mode of YHV98-1 yielded by induced-fit docking. **c** The simulation system of the YHV98-1 bound Hv1 channel. YHV98-1 is shown in blue spheres, Hv1 is shown in pink cartoon, and POPC in grey sticks. Water molecules, Na^+ and Cl^- are omitted for clarity. **d** Left, typical binding pose observed in the MD simulation; Right, the time-dependent distances between YHV98-1 and key residues involved in interactions. For clarity, only YHV98-1, water molecules and the interacting residues are shown. **e** Binding free energy decomposition of key residues in YHV98-4/Hv1 complex. Residues with energy contribution beyond -3 KJ/mol were highlighted in pink.