Table S1. Composition of the bilayer systems.

Model	Lipid types		Ion types		Peptide	Water	Initial system size [x,y,x; Å]	Simulation time [μs]
	Outer	Inner	Na^+	Cl^-				
No peptide	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	284	248	-	22112	117,117,200	5
TAT_1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	213	186	1	16254	117,117,150	10
TAT_15	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	248	302 347*	10 15*	21935 21853*	117,117,200	1 9
PTD4_1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	218	186	1	16301	117,117,150	10
PTD4_15	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	76 POPC 48 POPE 10 POPS 40 CHOL 18 DPSM 8 DPG1	248	252 272*	10 15*	22002 21949*	117,117,200	1 9

* Number of peptide molecules, chloride ion and water molecules after adding additional five peptide molecules to the system after 1 μs of the CG MD simulation. The CG MD simulations were then continued for another 9 μs.

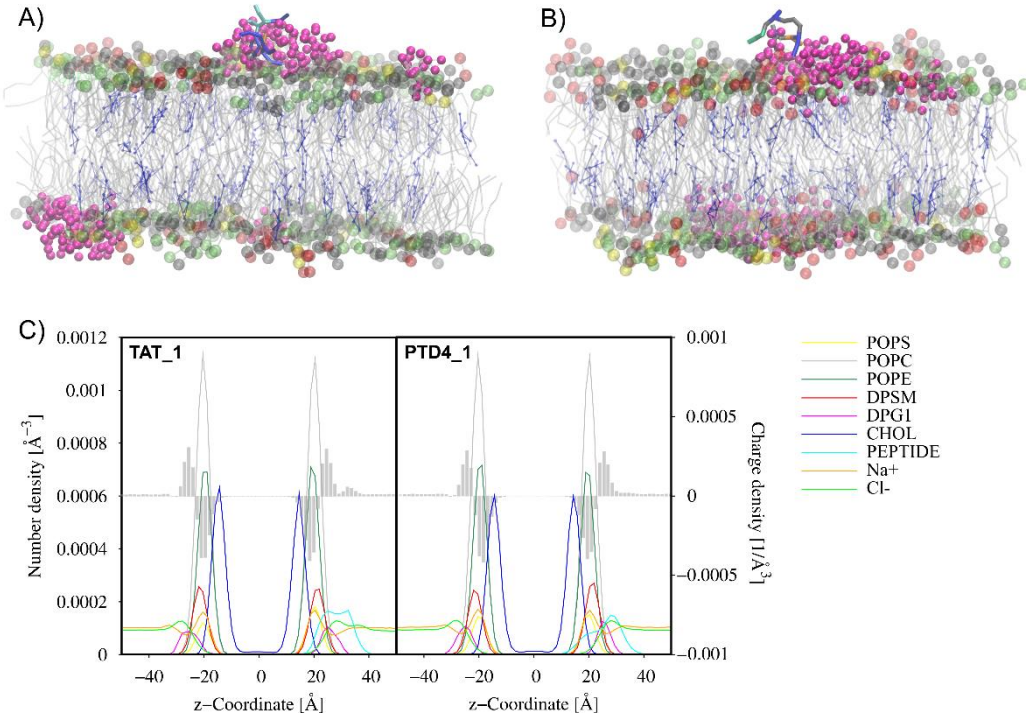

Figure S1. The final snapshots from the POPC:POPE:POPS:DPG1:DPSM:CHOL binding CG MD simulations for systems with a single molecule of Tat(49-57)-NH_2 (A) and PTD4 (B). The headgroups of POPC, POPE, POPS and DPSM are colored gray, lime, yellow and red, respectively. The sugar part of DPG1 is in magenta, while lipid acyl chains are presented in grey. CHOL is presented in blue as CPK model. (C) Partial density and charge density profiles averaged over the last 1 μs of MD CG simulations of the systems with a single peptide molecule.