SUPPLEMENTARY MATERIALS

Table S1. Details of MD trajectories discussed in the articles

Systems[a]	Length of MD, ns[b]	Abbreviations[c]	Comments
$DOPS_{128}$ / $water_{5624}$ / Na^{+}_{128}	15	*PS-pure*	The average A_L value is 63.3 Å^2
$DOPC_{128}$ / $water_{4821}$	20	*PC-pure*	The average A_L value is 70.2 Å^2
pAntp / $DOPS_{128}$ / $water_{5065}$ / Na^{+}_{121}	24	*PS-run1*	Non-polar residues of pAntp is oriented towards the membrane, basic and aromatic residues facing the water phase
pAntp / $DOPS_{128}$ / $water_{5065}$ / Na^{+}_{121}	24	*PS-run2*	Basic and aromatic residues of pAntp oriented towards the membrane, non-polar residues facing the water phase
pAntp / $DOPC_{128}$ / $water_{7060}$ / Cl^{-}_{7}	24	*PC-run1*	-/-
pAntp / $DOPC_{128}$ / $water_{7060}$ / Cl^{-}_{7}	24	*PC-run2*	-/-

[a] pAntp, penetratin (sequence, RQIKIWFQNRRMKWKK – basic residues are given with bold characters, non-polar and aromatic ones are underlined); subscripts correspond to the number of lipid or water molecules, and Na+ or Cl- counterions in the system.

[b] All MD trajectories were recorded with 0.002 ns separation time between system snapshots

[c] MD simulations of PS/PC-pure and PS/PC-run1/2 systems were carried out as described in Polyansky, A. A. et al., *J. Phys. Chem. B* **2005**, *109*, 15052-15059 and the first article of this series.

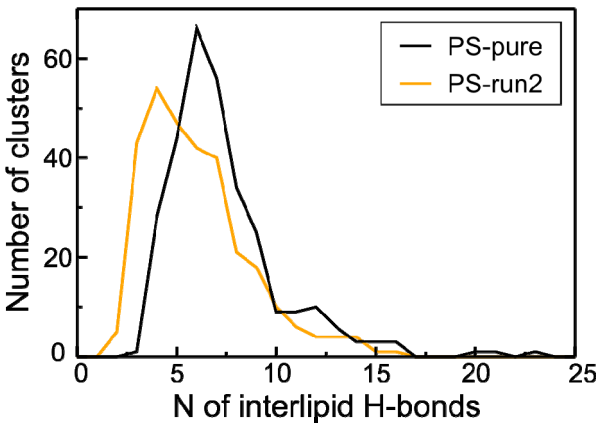

Figure S1. Histograms of H-bond cluster sizes (numbers of interlipid H-bonds) on the interface of "pure" DOPS bilayer and with the presence of pAntp. Statistics for the last 1 ns of MD is given. Delineation of H-bond clusters was carried out with the similar approach as for hydrophobic ones (*see Methods*). For the peptide-bilayer complex the data are shown only for the neighboring leaflet.