Electronic Supplementary Material (ESI) for Soft Matter.

ELECTRONIC SUPPLEMENTARY INFORMATION

Resolving the Structural Interactions between Antimicrobial Peptides and Lipid Membranes using Small-angle Scattering Methods: the case of Indolicidin

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1. Form Factor of asymmetric flat lipid bilayer:

The form factor for asymmetric flat lipid bilayers is given by

$$\mathrm{F}_{cos}(q) = \Delta\rho_{HG}\left(c_{HG_i}\sigma_{HG_i}\cos\left(qz_{HG_i}\right)\cdot\exp\left[-\right.\right.$$

(S1)

$$\mathrm{F}_{sin}(q) = \Delta\rho_{HG}\left(c_{HG_i}\sigma_{HG_i}\sin\left(qz_{HG_i}\right)\cdot\exp\left[-\left(\right.\right.\right.$$

$$q^{-1}\Delta\rho_{MN}\left[1-\frac{\pi^2\cos\left(q\sigma_{MN_i}\right)\cos\left(qz_{MN_i}\right)}{-\pi^2-4q^3\sigma_{MN_i}^2}\right]+\left(-\right.$$

$$\left.\left[1-\frac{\pi^2\cos\left(q\sigma_{MN_o}\right)\cos\left(qz_{MN_o}\right)}{-\pi^2-4q^3\sigma_{MN_o}^2}\right]\right.$$

(S2)

where σ_n and z_n are the width and position of the distribution respectively and $c_n = V_n/(A_L\sigma_n)$. V_n is the volume of the group n and A_L is the area per lipid, which is equal to the integrated area under the curve (n = HG (inner and outer), CG (inner and outer) , MN (inner and outer) and M).

2. Calculation of fraction of peptides in hydrocarbon tail region:

The integrals in Eq. 26 used to find the area of the overlap of the peptide Gaussian function and the hydrocarbon Gaussian function were derived to be the following:

$$\int_{z_p-5\sigma_p}^{z_{inter}} P_p = -\frac{c_p}{2}\sigma_p\mathrm{erf}\left(\frac{z_p - z_{inter}}{\sqrt{2}\sigma_p}\right)+\frac{c_p}{2}\sigma_p\mathrm{erf}\left(\frac{5\sigma_p}{\sqrt{2}\sigma_p}\right) \quad \text{(S3)}$$

$$\int_{z_{inter}}^{z_{MN_o}+\sigma_{MN_o}} P_{HC} = \frac{2\left(K_1\left(z_{MN_o}+\sigma_{MN_o}\right)+K_2\right)+\sin\left(2\left(K_1\left(z_{MN_o}\right.\right.\right.}{4K_1} \quad \text{(S4)}$$

where the two constants are defined as

$$K_1 = \pi/4\sigma_{MN_o} \quad \text{(S5)}$$

and

$$K_2 = \pi(-z_{MN_o}+\sigma_{MNo})/(4\sigma_{MN_o}) \quad \text{(S6)}$$

3. Fit parameters for neat liposomes with altering charge density:

Amount of negative lipids	2.5%	10%	15%	25%§	35%
Radius	*350*	*262*	*455*	*450*	*470*
Area	*60.4**				
z_{CH3}	*0**				
z_{CH2o}	*14.1 ±0.2***				
z_{CH2i}	*-13.8±0.2***				
z_{CGo}	*16.1±0.4***				
z_{CGi}	*-15.7±0.4***				
Z_{HGo}	*19.5±0.2***				
Z_{HGi}	*-19.3±0.2***				
σ_{CH3}	*2.3**				
σ_{CH2}	*4.9±0.3*				
σ_{CG}	*2±0.2*				
σ_{HG}	*4.1±0.5*				
DB	*38.8*				
DC	*11.7*				
VL	*1123*	*1106*	*1105*	*1099*	*1098*
V_{CH2}	*24.5*	*24.4*	*24.6*	*24.4*	*24.4*
V_{CG}	*153**				
V_{HG}	*176*	*165*	*158*	*157*	*155*
Rg PEG	*15**				
dcorr	*-10*	*-12*	*-8.2*	*-8.6*	*-11*
σ_{SD}	0.3	0.3	0.33	0.35	0.24

*Table S1 Fit parameters for liposomes with altering amount of negatively charged liposomes as indicated in the table. Hard constrained parameters are designated by * and soft constrained by limits in fitting regime indicated by **. The units for all numbers carry the appropriate power of Å. §For this sample a joint fit analysis of SAXS and SANS data was performed.*

4. Fit with symmetric model:

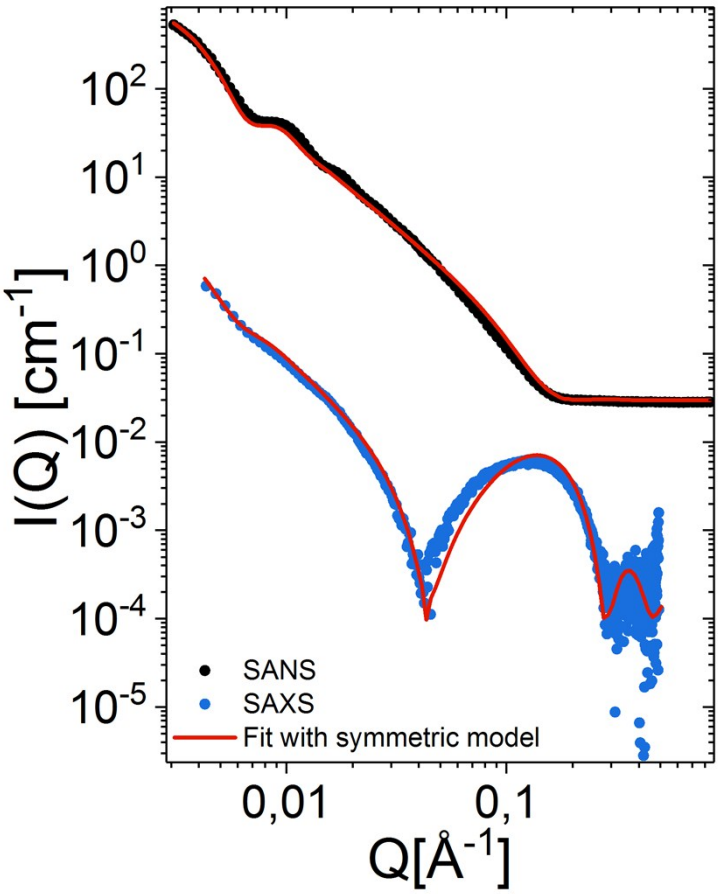

Figure S1 Neutron and x-ray scattering plot for DMPC-DMPG 25 % liposomes and the joint fit using a symmetric bilayer model. As seen from the figure the symmetric bilayer model has a deeper minimum at intermediate q than the experimental data and, consequently, a slight asymmetry was introduced.