Electronic Supplementary Material (ESI) for Soft Matter

Modulating the structure and interactions of lipid–peptide complexes by varying membrane composition and solution conditions

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Supporting information

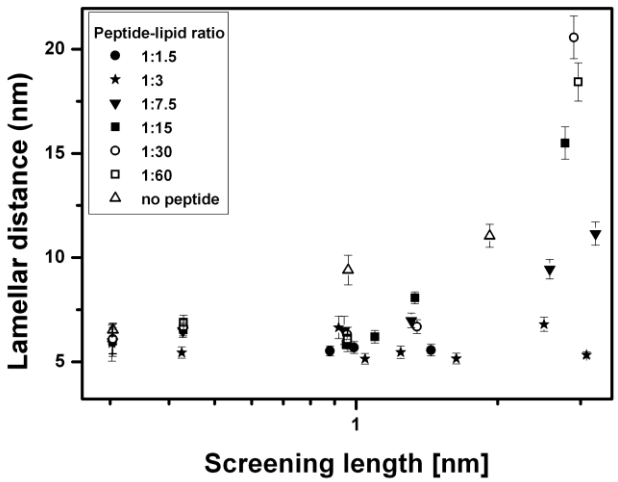

Figure S1: The region of short screening lengths of Figure 4 on an expanded scale. Lamellar repeat distance of the Caco-2 model membrane as a function of the screening length (taking into account both NaCl and peptide concentrations), at a variety of peptide-lipid molar ratios.

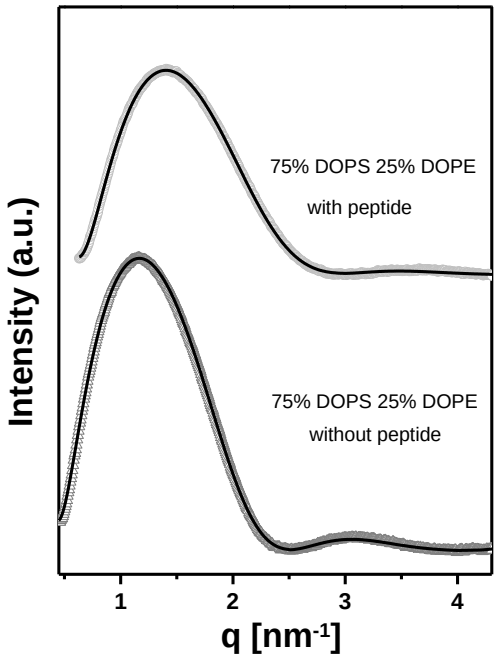

Figure S2. Form factor of 75% DOPS and 25% DOPE membrane with (top) and without (bottom) the peptide at P/L = 1:3. No salt is added. The parameters of the best fitted models (eq. 8) are shown in Table S1.

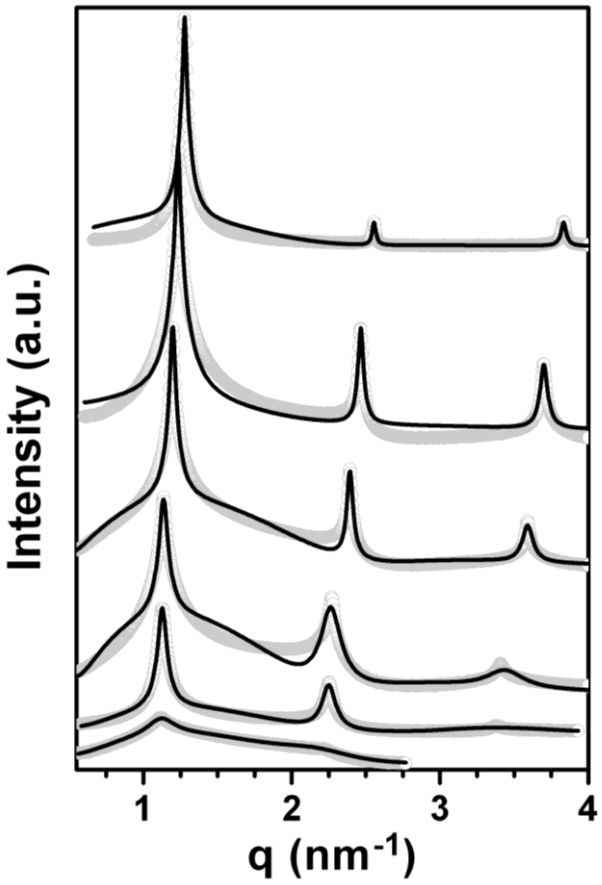

Figure S3. Radially averaged scattering intensities of lipid-peptide complexes at a peptide-lipid molar ratio of 1:3, at different membrane compositions (open symbols). All the membranes contain DOPS molar fraction of 0.15, and the zwitterionic lipids DOPC and DOPE comprise the rest of the membranes. Molar fractions of DOPE from top to bottom: 0.85, 0.7, 0.55, 0.35, 0.15. The very last bottom curve corresponds to 15% DOPS and 85% DOPC. Solid curves corresponds to simulated structure factor (eq. 8), using the best fitted model parameters, shown in Table S1, Figure S4, and Figure S5.

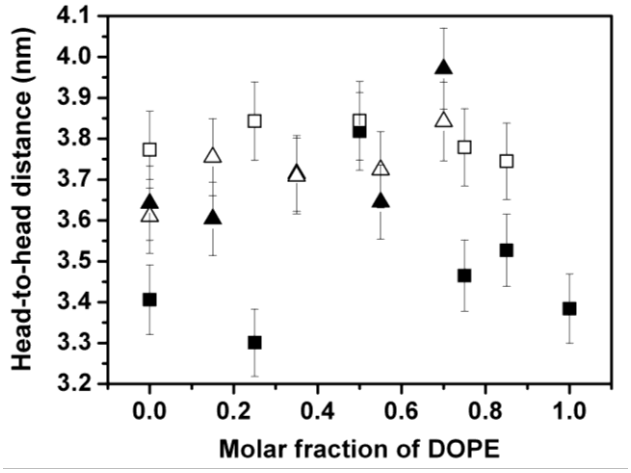

Figure S4. Head to head distance of membrane – peptide complexes as a function of the DOPE molar fraction. Solid symbols correspond to membrane – peptide complexes, peptide to lipid molar ratio, P/L = 1:3, open symbols correspond to the case of no added peptides (i.e. the membranes alone). Square symbols – membranes with DOPE and DOPS only. Triangles – DOPE/DOPS/DOPC membranes with 0.15 molar fraction DOPS, DOPE as indicated in the figure, and the remaining lipid molar fraction is DOPC. Data are also presented in Table S1.

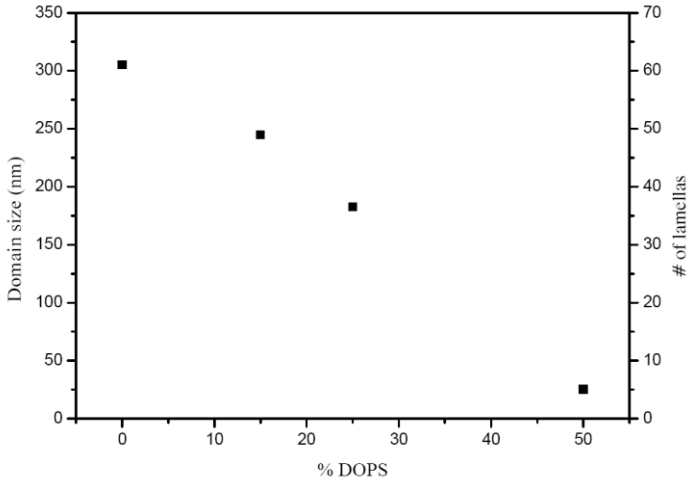

Figure S5. The number of layers in the multi-lamellar phase or domain size as a function of the amount of DOPS in DOPS/DOPE membranes with peptide at P/L of 1:3, based on line-shape analysis of the data in Figure S3.

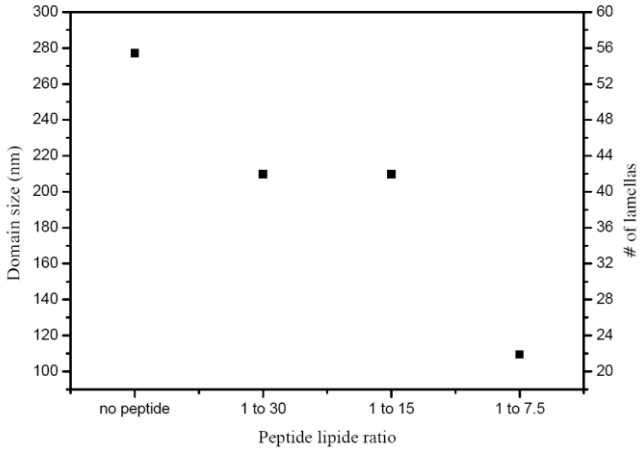

Figure S6. Number of lamellas and domain size as a function of peptide to lipid molar ratio for DOPC membranes, based on line-shape analysis of the data in Figure 8.

Table S1: Length and electron density of the head group, carbon tails and the full head-to-head length of the different membranes. All the data were fit to Eq. 8 using X+. The rows in gray are samples with the peptide at P/L=1:3, the other samples are of membranes with no added peptide. Error in tail length is ~0.5%, error in head size and in electron density is <1.5% and error in head-to-head <2.5%.

	Membrane composition			Carbon tail length (nm)	Head length (nm)	Tail electron density (e/nm^3)	Head electron density (e/nm^3)	Head-to-head distance (nm)
	%DOPS	%DOPE	%DOPC					
no PEP	15	0	85	1.163	1.284	271	388	3.61
PEP	15	0	85	1.371	0.9	290	405	3.642
no PEP	50	0	50	1.115	1.34	275	391	3.57
PEP	50	0	50	0.907	1.359	267	403	3.173
no PEP	75	0	25	1.272	1.336	294	410	3.88
PEP	75	0	25	0.989	1.383	284	392	3.361
no PEP	100	0	0	1.193	1.387	276	411	3.773
PEP	100	0	0	1.004	1.398	281	402	3.406
no PEP	15	15	70	1.157	1.441	265	414	3.755
PEP	15	15	70	1.015	1.574	288	385	3.604
no PEP	75	25	0	1.191	1.461	286	387	3.843
PEP	75	25	0	0.96	1.381	289	389	3.301
no PEP	15	35	50	1.241	1.226	278	399	3.709
PEP	15	35	50	1.236	1.243	276	405	3.715
no PEP	50	50	0	1.193	1.458	266	408	3.844
PEP	50	50	0	1.176	1.466	295	402	3.818
no PEP	15	55	30	1.206	1.312	283	396	3.724
PEP	15	55	30	1.073	1.499	267	408	3.645
no PEP	15	70	15	1.252	1.338	277	403	3.842

PEP	15	70	15	1.312	1.347	276	414	3.971
no PEP	25	75	0	1.201	1.377	271	401	3.779
PEP	25	75	0	1.09	1.285	291	393	3.465
no PEP	15	85	0	1.174	1.397	268	403	3.745
PEP	15	85	0	1.029	1.469	275	394	3.527
no PEP	0	100	0	0.916	0.974	275	389	2.806
PEP	0	100	0	1.205	0.974	291	385	3.384
no PEP	25	0	75	1.16	1.329	265	411	3.649