Supporting Information

On the destabilization of lipid membranes by a peptide derived from glycoprotein gp36 of feline immunodeficiency virus: a combined molecular dynamics/experimental study.

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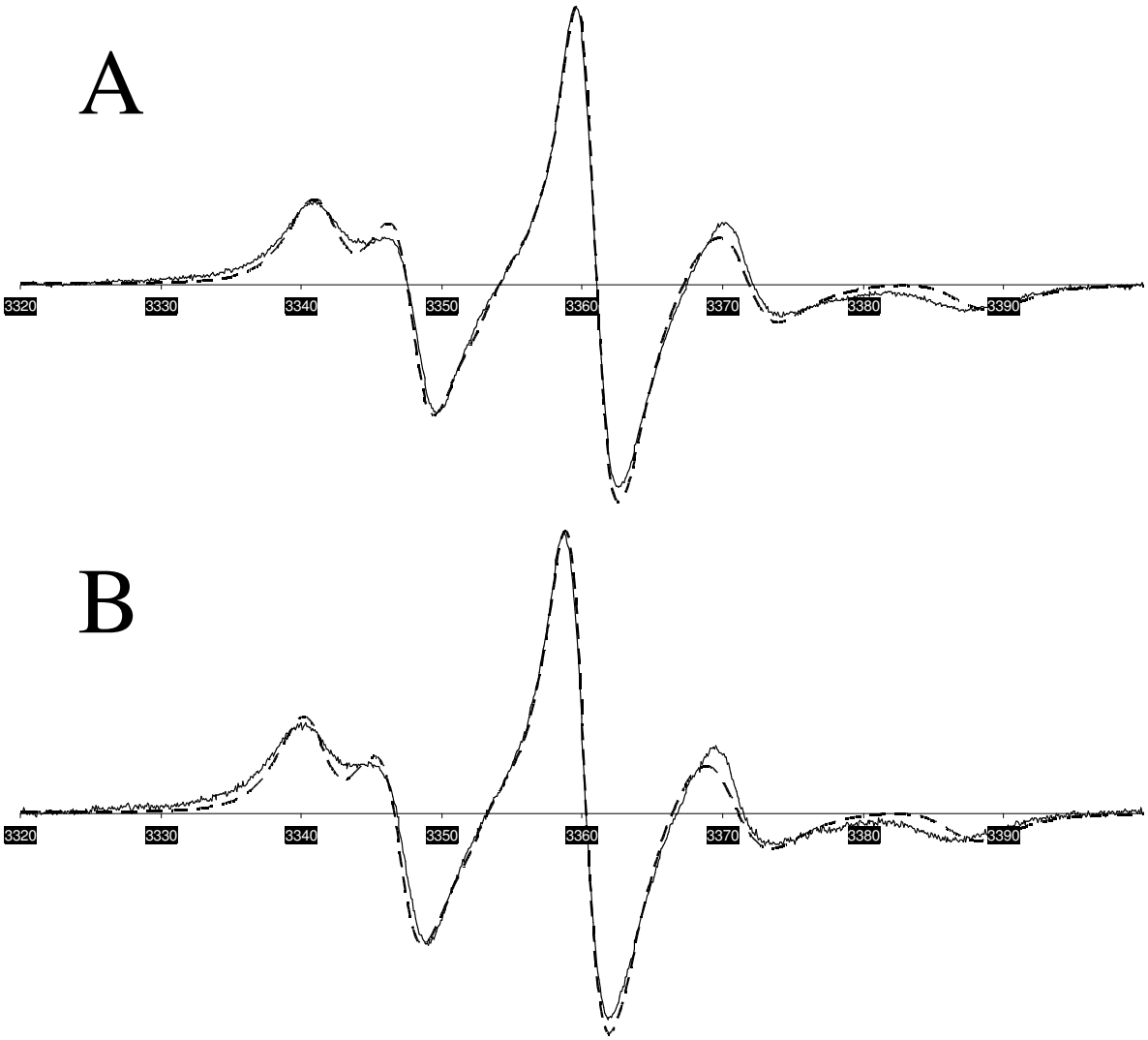


Fig. S1 ESR spectra of 5-PCSL in POPC bilayers at 37 °C in the absence (A) and in the presence (B) of 0.5:1 wt/wt C8 peptide 1 (continuous lines) paired with their best simulation (dashed lines).

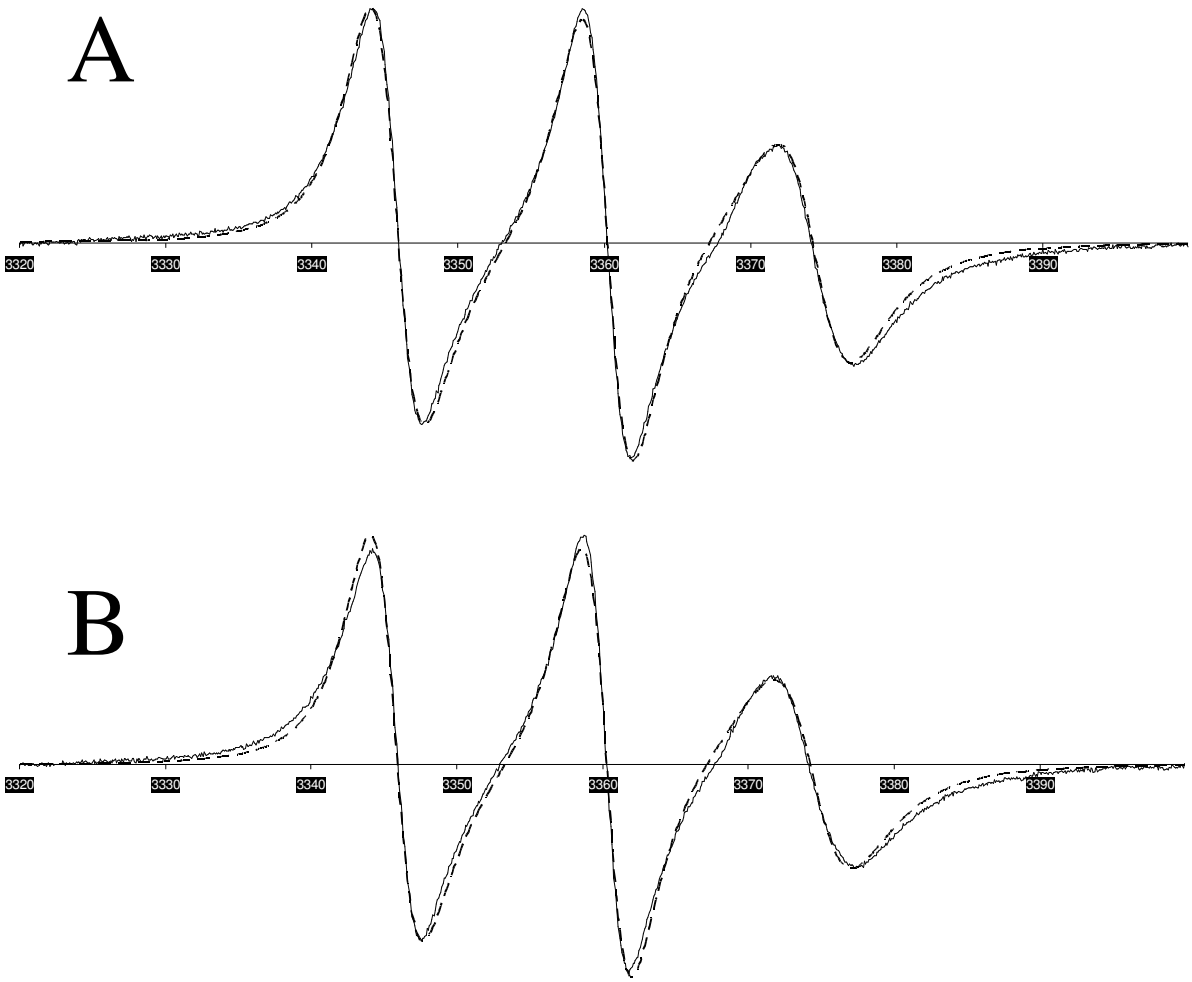
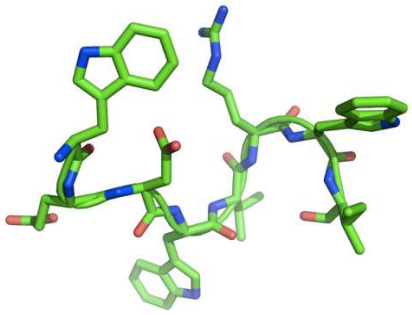


Fig. S2 ESR spectra of 5-PCSL in POPC bilayers at 37°C in the absence (A) and in the presence (B) of 0.5:1 wt/wt C8 peptide 1 (continuous lines) paired with their best simulation (dashed lines).

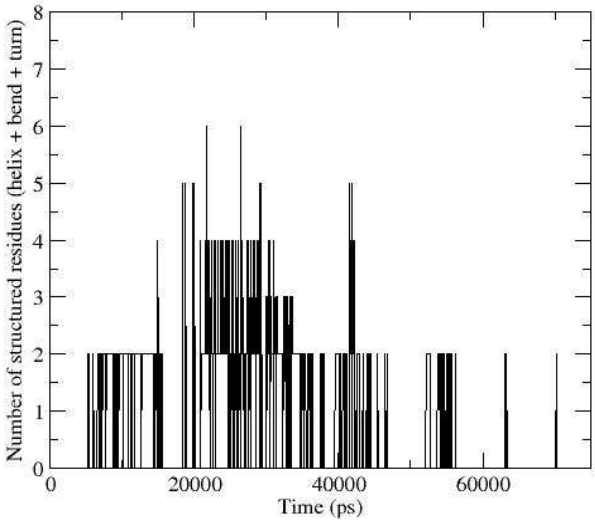
Table S1 Magnetic and dynamic parameters derived from the simulation of the ESR spectra of 5-PCSL and 14-PCSL in POPC bilayers, in the absence and in the presence of the C8 peptide.

	POPC	**POPC-C8**	**POPC**	**POPC-C8**
	5-PCSL		**14-PCSL**	
g_{xx} (±0.0002)	2.0100	2.0100	2.0186	2.0186
g_{yy} (±0.0002)	2.0088	2.0086	2.0001	2.0001
g_{zz} (±0.0002)	2.0054	2.0053	2.0058	2.0058
A_{xx} /G (±0.2)	2.8	2.9	6.9	7
A_{yy} /G(±0.2)	12.6	12.3	10.7	10.6
A_{zz} /G(±0.2)	27	27.1	21.5	21.3
$\tau_{(C)}$xx /ns (±1)	139	163	19	24
$\tau_{(C)}$yy /ns(±1)	7	7	2	3
$\tau_{(C)}$zz /ns(±1)	5	5	2	2

A



B



C

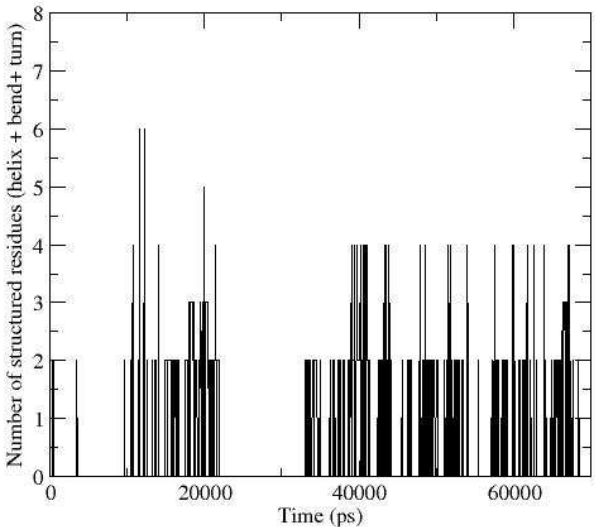


Fig. S3 A) Representation of the peptide conformation derived from NMR measurements (Ref. 44). Time evolution of the number of residues in α-helix, bends and turns as function of time in the simulations of C8 in water; B) results from the simulation starting with the NMR structure, C) results from the simulation starting with a random structure. In both cases, C8 appears to have a low tendency to form a well defined structure.

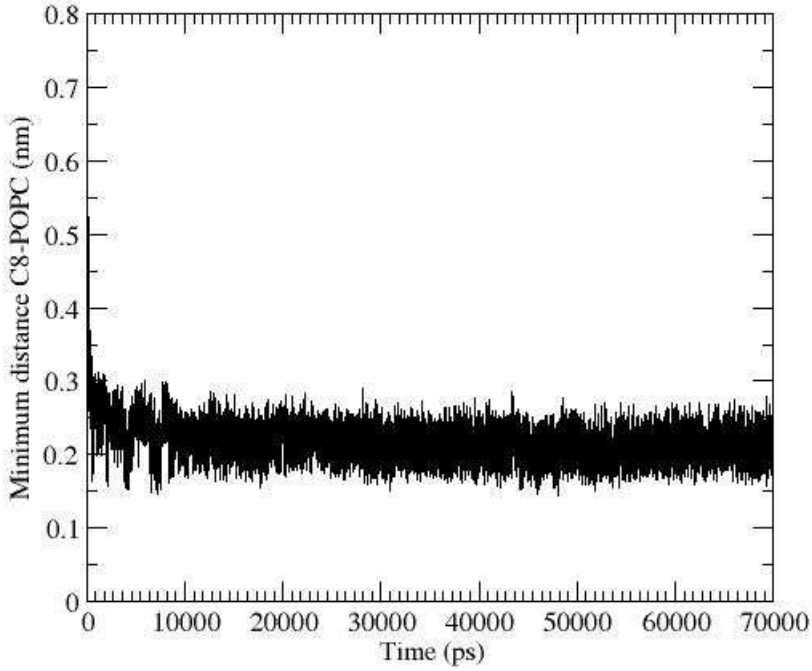


Fig. S4 The minimum distance between C8 and POPC during the simulation. The distance is calculated between the centre of mass of C8 and the closest atoms of POPC.

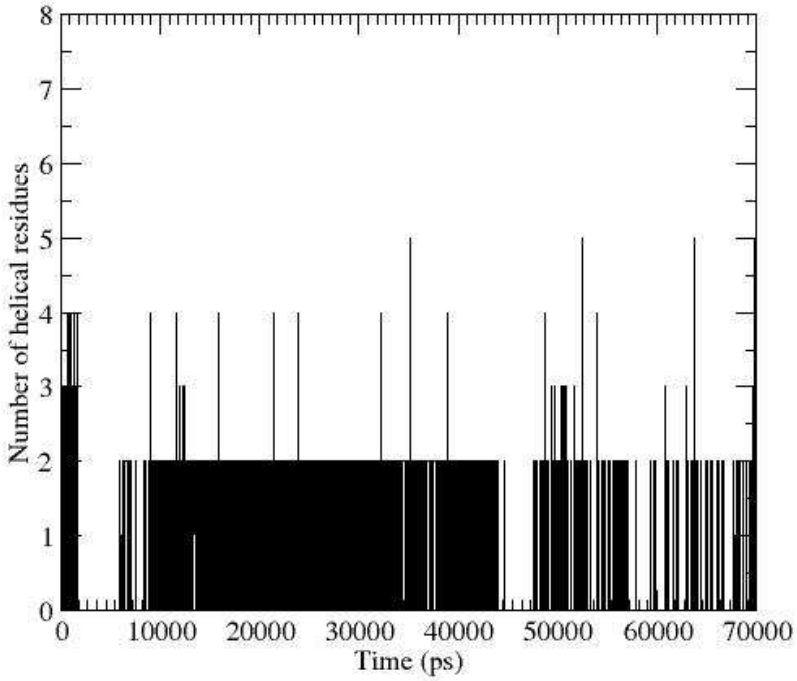


Fig. S5 Number of residues in helical conformation during the simulation.

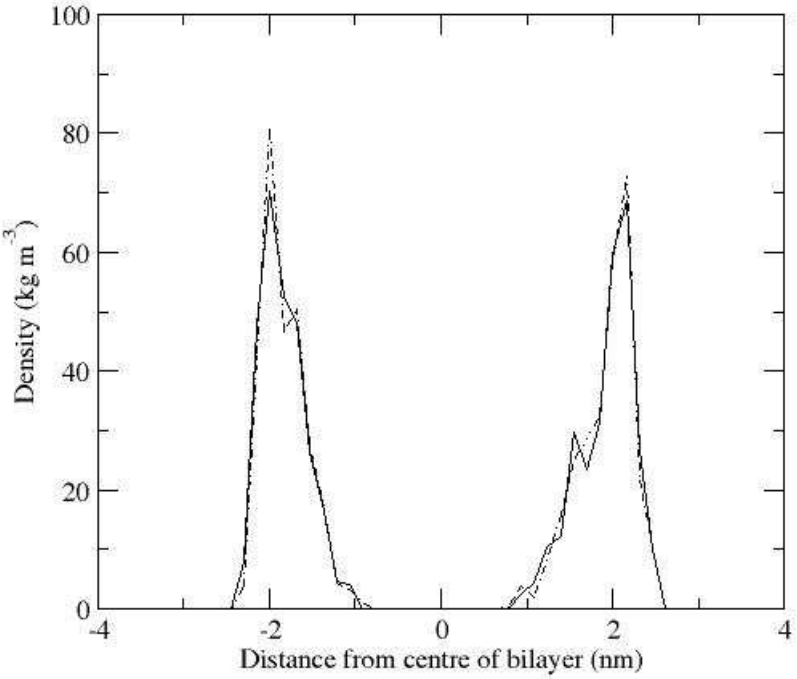


Fig. S6 Density profile of the phosphorus atoms before (solid lines) and after peptide (dashed lines) the binding of the C8 peptide.

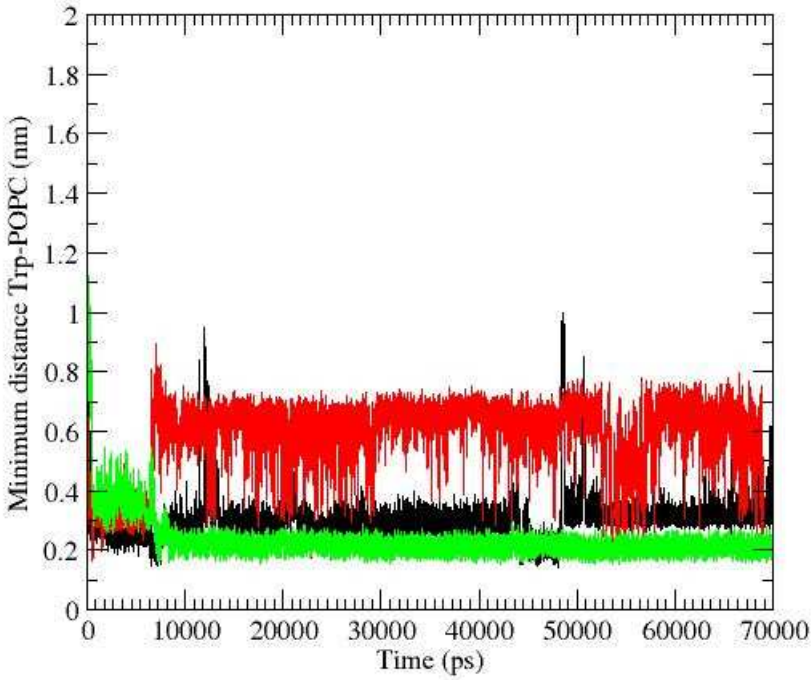


Fig. S7 The interactions between Trp residues and POPC molecules. Green lines represent the minimum distance between Trp776 and POPC, black lines the distance between Trp770 and POPC and red lines that between the Trp773 and POPC.

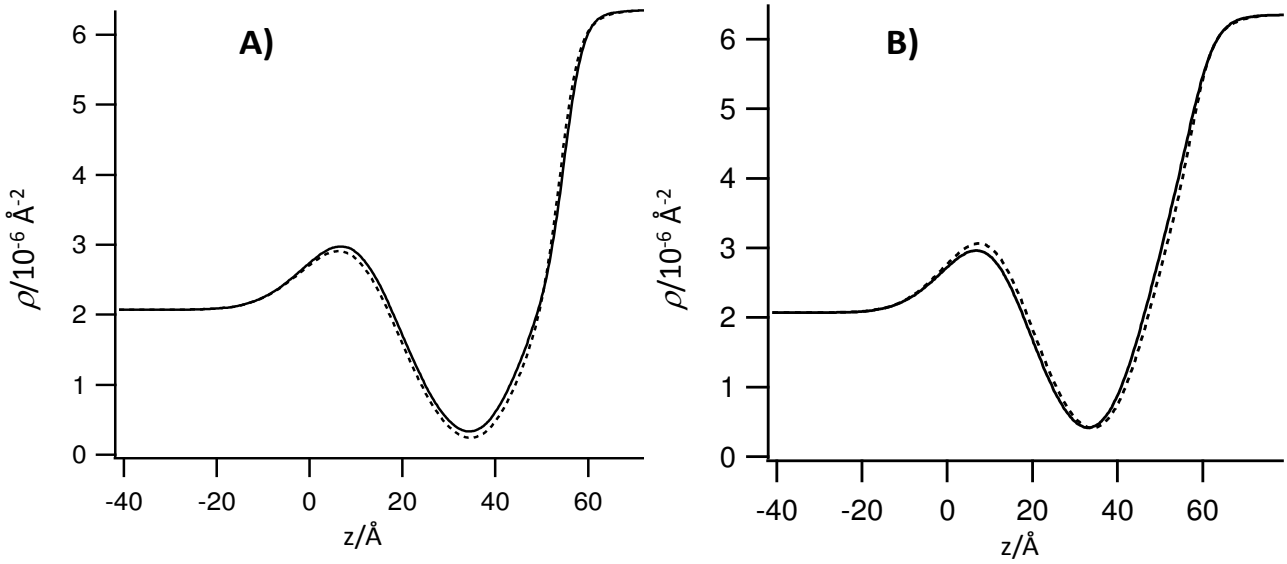


Fig. S8 – Comparison between the scattering length density, $\rho(z)$, profile of pure POPC (**A**) and POPC with C8 (**B**) bilayers, obtained by experimental (continuous line) and computational (dotted line) data. The thickness of the chains region, headgroups and interacting peptide layers has been estimated from the MD simulations as follows atoms of the: the chains region thickness has been calculated as the average distance between the carbons in α to the carboxylic groups of the lipid acyl chains of the two opposing leaflet. The headgroups layers thickness has been calculated by subtracting the thickness of chains region to the average distance between the nitrogen atoms of the choline groups of the two opposing leaflets. The thickness of the interacting peptide layer has been calculated as the average distance between the peptide atoms closest and farthest to the lipid headgroups. These thickness values are reported in Table S2.

Table S2 Neutron reflectivity and MD calculated thickness of the layers in which a POPC bilayer, in the absence and in the presence of interacting C8 peptides, can be conceptually sectioned:

	Calculated data/Å*	Experimental data/Å*
POPC bilayer		
Chain region	30.4 (0.6)	28(1)
Outer headgroup	6.4 (0.6)	8(1)
POPC bilayer after C8 binding		
Chain region	30.8 (0.6)	31(1)
Outer headgroup	4.7 (0.6)	5(1)
Interacting peptide	4.7 (0.6)	5(1)

*Errors in parenthesis