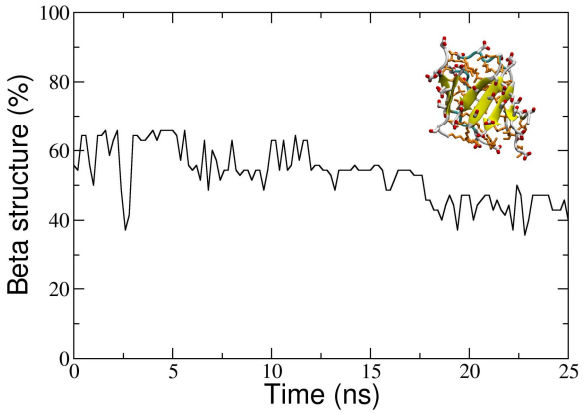
Table S1. Atomistic and coarse-grained simulations carried out for the ADA8 peptide. Simulations CG3 and CG 6 have also been carried out for the ABZ12 peptide.

Run	System	Box size (nm)	Simulation time (ns)
AT1	$Peptide_1/Water_{11448}$	5.1 x 5.1 x 3.6	3 x 50
AT2	$Peptide_{10}/Water_{32443}$	10.0 x 10.0 x 10.0	3 x 1,000
CG1	$Peptide_1/Water_{936}$	3.9 x 2.7 x 3.3	3 x 10
CG2	$Peptide_{10}/Water_{7540}$	10.0 x 10.0 x 10.0	3 x 10,000
CG3	$BRD^1/Peptide_{10}/Water_{7206}$	10.0x10.0x10.0	3 x 25,000
CG4	$BRD^1/DPC_{150}/Water_{6518}$	10.0x10.0x10.0	3,000
CG5	$BRD^1/DPC_{104}/Water_{4852}$	9.0x9.0x9.0	1,000
CG6	$BRD^1/Peptide_{20}/DPC_{104}/Water_{12538}$	11.0 x 11.0 x 11.0	3 x 25,000



[1] BRD= bacteriorhodopsin protein

Figure S1. The secondary structure evolution of the ADA8 peptide after a reverse transformation from coarse grained to atomistic resolution. Insets show the structures at the end of the simulations.

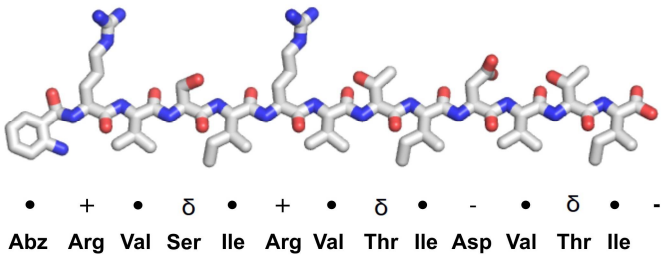


Figure S2. The sequence, properties and structure of peptide sABZ12 at neutral pH. ●, +, δ and - represent hydrophobic, positively charged, polar and negatively charged residues, respectively. Abz, Ac and Am correspond to the aminobenzoyl group, acetylation and amidation, respectively.

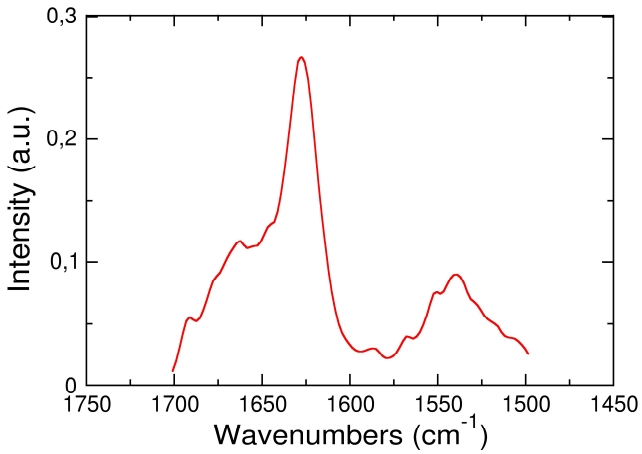


Figure S3. ATR-FTIR spectrum of the amide I band of the ABZ12 peptide. 200 μg of peptides have been dissolved at 1% weight/volume in DMSO.

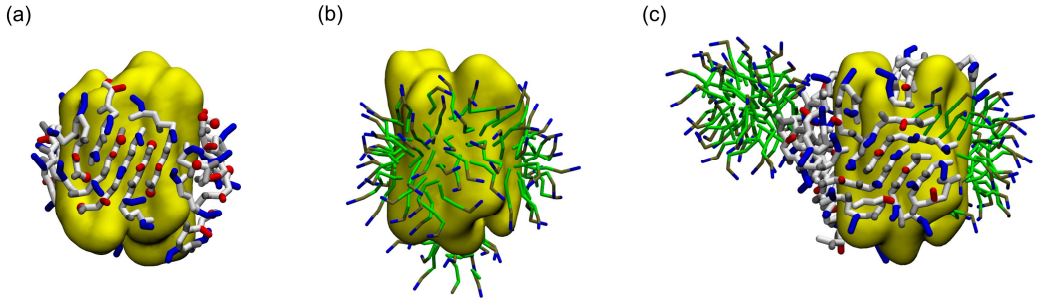


Figure S4. ABZ12 peptide organization on the surface of the membrane protein. The structures show 20 peptides at the end of the CG simulations when the protein (in yellow) is alone (a) or initially covered by DPC (c). The protein in a micelle of DPC is shown (b), and this structure was used as a starting point before the addition of the peptides (c).

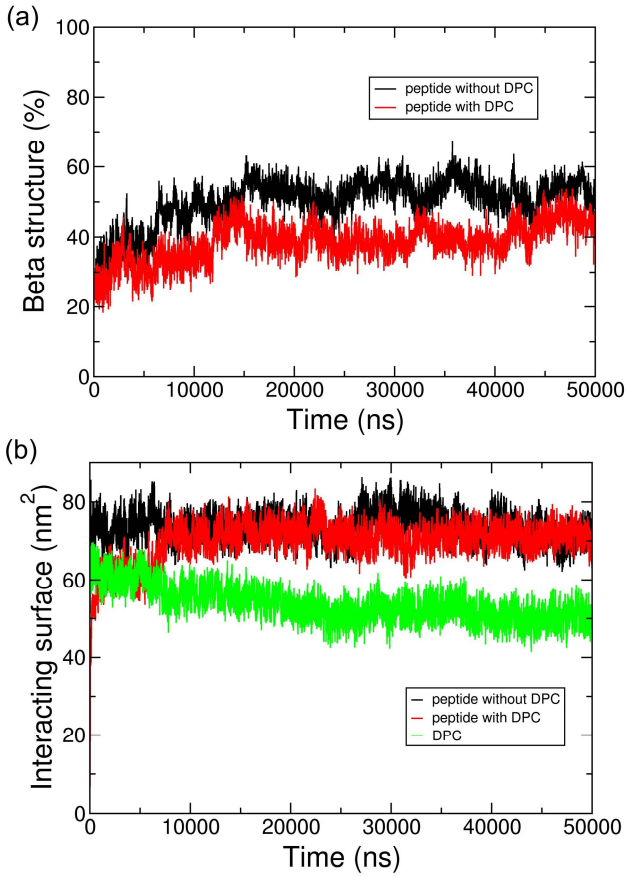


Figure S5. The secondary structure evolution (a) and surface of the interaction (b) of the peptide ABZ12 in the presence of a membrane protein with (red lines) and without (black lines) DPC. The surface of the interaction between DPC and the membrane protein in the presence of the ABZ12 peptide is represented in green.