Supplementary Materials

Antimicrobial peptide K11 selectively recognises bacterial biomimetic membranes and acts by twisting their bilayers

Francisco Ramos-Martín, Claudia Herrera-León, Viviane Antonietti, Pascal Sonnet, Catherine Sarazin, and Nicola D'Amelio

Family members coloured by frequency:

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22. Leukemia Cancer(IC50=100 µM), Lung Cancer(IC50=100 µM), Blood Cancer(IC50=75 µM), Breast Cancer(IC50=100 µM), Human, Escherichia coli KCTC 1682(MIC=3.125 µM), Salmonella typhimurium KCTC 1926(MIC=0.78 µM), Pseudomonas aeruginosa KCTC 1637(MIC=0.78 µM), Bacillus subtilis KCTC 1918(MIC=0.78 µM), Streptococcus pyogenes KCTC 3096(MIC=0.78 µM), Staphylococcus aureus KCTC 1621(MIC=3.125 µM), Staphylococcus aureus (MIC=3 µM), Escherichia coli(MIC=3 µM), S. typhimurium

 Lung Cancer(ICS0=2.5, µM), Lung Cancer(ICS0=2.3, µM), Lung Cancer(ICS0=3, µM), Escherichia Coli(mIC=2, µM), Escherichia Coli(mIC=2, µM), Lung Cancer(ICS0=1.6, µM), Lung Cancer(ICS0=5, µM), Blood Cancer(ICS0=30, µM), Breast Cancer(ICS0=4, µM), Lung Cancer(ICS0=5, µM), Lung Cancer(ICS0=5, µM), Blood Cancer(ICS0=30, µM), Breast Cancer(ICS0=4, µM), Lung Cancer(ICS0=5, µM), Lung Cancer(ICS0=16, 1, µM), Lung Cancer(ICS0=16, 1, µM), Lung Cancer(ICS0=5, µM), Blood Cancer(ICS0=10, µM), Blood Cancer(IHC=10, µM), Gastric Cancer(IHC=10, µM), Sathrana(IHC=25, µM), Human(IHC=25, µM), Human(IHC=25, µM), Bacillus subtilis KCTC 1918(MIC=0, 78, µM), Streptococcus pyogenes KCTC 3096(MIC=0, 78, µM), Staphylococcus aureus KCTC 1621(MIC=3, 125, µM), Escherichia coli KCTC 1637(MIC=0, 78, µM), Bacillus subtilis KCTC 1918(MIC=0, 78, µM), Streptococcus pyogenes KCTC 3096(MIC=0, 78, µM), Staphylococcus aureus KCTC 1621(MIC=3, 125, µM), Escherichia coli KCTC 1637(MIC=0, 78, µM), Staphylococcus aureus KCTC 1621(MIC=3, 125, µM), Staphylococcus aureus KCTC 1621(MIC=3, 125, µM), Escherichia coli KCTC 1637(MIC=0, 78, µM), Staphylococcus aureus KCTC 1621(MIC=3, 125, µM), Staphylococcus aureus KCTC 1621(M 1637(MIC=1.56 μM), Bacillus subtilis KTCT 1918(MIC=0.78 μM), Streptococcus pyogenes KTCT 3096(MIC=0.78 μM), Staphylococcus aureus KCTC 1621(MIC=3.125 μM), Escherichia co ATCC 33694(MIC=6.25 μM), Bacillus subtilis ATCC 6633(MIC=1.56 μM), Human lung carcinoma NCI-H146(ICS0=13 μM), Human lung carcinoma NCI-H126(ICS0=16 μM), Acinetobacter baumannii (MIC=12.5 μM), Streptococcus epidermidis KCTC 3096(MIC=3.12 μM), Candida albicans TIMM 1768(MIC=12.5 μM), Trichosporon beigelii KCTC 7707(MIC=6.25 μM), Escherichia coli CCARM 1229(MIC=8 μM), Escherichia coli CCARM 1229(MIC=8 μM), Pseudomonas aeruginosa 3552(MIC=4 μM), Staphylococcus aureus 3518(MIC=2 μM), Staphylococcus aureus 3518(MIC=64 μM), Staphylococcus aureus 1870(MIC=64 μM), Staphylococcus aureus 4716(MIC=4 μM), Staphylococcus aureus 3515(MIC=1 μM), Staphylococcus aureus 4716(MIC=4 μM), Staphylococcus aureus 3515(MIC=1 μM), Staphylococcus aureus (MIC=3 μM), Buchholderia pseudomallei, Escherichia coli(MIC=3 μM), Beadomonas aeruginosa(MIC=2 μM), St. typhimurium Lung Canceri(ICS0=3 1 μM), Staphylococcus aureus 3516(MIC=4 μM), Staphylococcus aureus 3516(MIC=4 μM), Staphylococcus aureus 3516(MIC=4 μM), Staphylococcus aureus 3516(MIC=3 μM), Buchholderia

25. Lung Cancer(IC50=3.1 μM), Lung Cancer(IC50=2.4 μM)

Lung Cancer(IC50=9.5 μM), Lung Cancer(IC50=10.9 μM)
Lung Cancer(IC50=1.9 μM), Lung Cancer(IC50=1.3 μM), Lung Cancer(IC50=2.8 μM)

Bacillus subtilis ATCC 9372(MIC=100 μM), Bacillus anthracis Sterne 34F2(MIC=100 μM), Burkholderia thailandensis(MIC=50 μM)
Lung Cancer(IC50=36.2 μM), Lung Cancer(IC50=37.9 μM), Lung Cancer(IC50=47.7 μM)

30. Lung Cancer(IC50=2.9 μM), Lung Cancer(IC50=3.2 μM)

Figure S1. (A) Sequence alignment of K11 peptide used as a bait in the ADAPTABLE web server. (B) ADAPTABLEgenerated consensus sequence and available data for the anticancer activity of each peptide of the family shown in (A).

B



Figure S2. (A-D) ¹H,¹³C-HSQC spectral regions and assignment of K11 in solution (blue and green for positive and negative signals respectively) and in the presence of DPC micelles (red and magenta for positive and negative signals respectively): aromatic region (A), magnification of Phe aromatic region (B), H β region (C) and side chain regions (D). (E-F) NOESY spectrum of K11 in the presence of DPC micelles showing meaningful NOEs in the aromatic/aliphatic (E) and amide (F) regions.



Figure S3. Minimum distance of each lysine side chain amine (atom name NZ) from membrane phosphorus atoms along the simulation trajectory of K11 interacting with DPC micelles.



Figure S4. ¹H NMR normalized spectra of K11 1mM in the presence of DMPC/DHPC (blue), DMPC/DHPC/DMPE (orange), DMPC/DHPC/DMPG (black), DMPC/DHPC/DMPS (green) bicelles at a total concentration 70 mM. The spectrum in the presence of DPC 60 mM (gray) is shown for comparison.



Figure S5. Occurrence of polar atom contacts (H-bonds and salt bridges) between K11 peptide and various membrane bilayers calculated along MD simulation trajectories.



Figure S6. Occurence of polar atom contacts (H-bonds and salt bridges) between K11 peptide and various membrane bilayers calculated along MD simulation trajectories. TOCL2 refers to CL.



Figure S7. Area per lipid (nm²) in bilayers containing various phospholipids compositions as calculated from MD simulations in the presence of eight K11 peptides. The average value is shown in blue while the upper and lower leaflet are shown in yellow and red respectively. TOCL2 refers to CL.



Figure S8. Order parameter of C-H moieties in palmitoyl side chains in membranes containing various phospholipids compositions as calculated from multiple repetitions of MD simulations in the absence (2 repetitions in black labeled as 1 and 2) and in the presence (3 repetitions in red labeled from 1 to 3) of eight K11 peptides. The panel in the right bottom corner is an example of MD snapshot with POPE/POPG bilayer (color code in the caption of Figure 4). TOCL2 refers to CL.



Figure S9. Electron density profiles for POPC (A), POPG (B) and POPE/POPG/CL (C) in presence of eight K11 peptides. TOCL2 refers to CL.



Figure S10. Order parameter of C-H moieties in palmitoyl side chains in membranes containing various phospholipids compositions as calculated from multiple repetitions of MD simulations in the absence (2 repetitions in black labeled as 1 and 2) and in the presence (3 repetitions in red labeled from 1 to 3) of K11 peptide initially placed inside the bilayer. The panel in the right bottom corner is an example of MD snapshot with POPE/POPG/CL bilayer (color code in the caption of Figure 4). TOCL2 refers to CL.



Peak Purity Index	Ret. Time	Area	Height	Area %	Height %	
200.	21.975	222959	18837	2.187	3.139	
	22.379	9970525	581156	97.813	96.861	
		10193484	599992	100.000	100.000	

Figure S11. Analytical purity of K11 peptide. HPLC C12 column (Phenomenex® C12, Jupiter 4 μ Proteo, 90 Å, 250x4.6 mm) using a mixture of aqueous 0.1% (v/v) TFA (A) and 0.1% (v/v) TFA in acetonitrile (B) as the mobile phase and employing UV detection at 210 nm.



Figure S12. Convergence analysis of the simulation of K11 peptide in the presence of POPE/POPG membrane. (A) Peptide RMSD ($C\alpha$ carbon); (B) Polar contact block analysis in time intervals.

	I VS1	TRP2	I VS2	SER/	PHES	II E6	I VS7	I VC8	I EI IO	THR10
ΊH	NH=X	NH=8 165	NH=8 17	NH=8 13	NH=8 395	5 NH=8 146	NH=8.48	NH=8 384	NH=8 56	NH=8.3
	α =3.914	α =4.63	α =4.16	α =4.188	α =4.63	α=4.06	α=4.24	α=4.2	α =4.45	α =4.325
	β1 = 1.818	β = 3.28	β1 = 1.6	β =3.75	β1 = 3.04	β=1.75	β = 1.76	β=1.7	β =1.57	β=4.2
	β ₂ =1.62	€1=10.23	β2 = 1.56		β2=3.09	γı=1.75	γ = 1.45	γ = 1.71	γ = 1.65	β2 =2.9 0
	γ = 1.395	€3 = 7.62	γ=1.24		δ=7.23	γ2 = 0.86	δı=1.45	δ=1.36	δ1=0.87	δ2=1.2
	δ= 1.7	δ =7.28	δ=1.62		€ = 7.4	δ=0.85	δ2=1.13	€ =?	δ2=0.95	
	€ = 2.97	ζ2=7.5	∈=?		ζ=7.4		€ = 3.07			
		ζ3 = 7.17								
		η2 =7.25								
¹³ C	α =55.94	<i>α</i> =58	<i>α</i> =56.14	α =58.25	α =57.9	α =61	α =56.5	α =56.5	α =55.17	<i>α</i> =62.1
	β =33.93	β=29.9	β=33.87	β=64	β=40	β =38.5	β=33.2	β=33.2	β = 42.58	β=70.2
	γ = 24.91	€3 = 120	γ = 24.7		δ=132	γ1 = 33.4	γ = 25	γ = 25	γ = 27.17	γ2 =21.8 1
	δ=29.44	δ1=127	δ=29.13		€ = 131	γ = 17.45	δ=27.5	δ=29.5	δ1 =23.65	
	€ = 42.2	ζ2 = 114.4	∈=?		ζ=130	δ1=12.8	€ = 42.2	€ = 42.2	δ2=25.15	
		ζ3 =122								
		η2 = 124								
	LYS11	LYS12	PHE13	LEU14	HIS15	SER16	ALA17	LYS18	LYS19	PHE20
¹ H	NH=8.54	NH=8.44	NH=8.46	NH=8.3	NH=8.43	NH=8.45	NH=8.54	NH=8.44	NH=8.54	NH=8.42
	$\alpha = 4.24$	α = 4.25	<i>α</i> =4.59	α =4.32	α = 4.6	α =4.4	α = 4.33	α = 4.25	$\alpha = 4.24$	α = 4.58
	β =1.74	β=1.7	β1 = 3.08	β=1.54	β =3.17	β =3.85	β=1.4	β =1.7	β =1.74	β1 = 3.04
	γ =1.4	γ = 1.315	β2=2.98	γ = 1.5	γ2 =7. 11			γ = 1.315	γ = 1.4	β2 = 3.14
	δ =1.67	δ=1.68	δ=7.21	δ ₁ =0.85	€ 1 = 8.07			δ=1.68	δ=1.67	δ=7.3
	€ = ?	€ = 3.1	ε =7.4	δ 2 =0.88				€ = 3.1	∈ =?	ϵ =7.4
			ζ=7.4							ζ=7.4
¹³ C	α =56.56	α = 56.5	α =57.7	α =55.1	α =56.5	α =58.4	α =52.7	α =56.5	α =56.56	α =57.77
	β=33.2	β=33.3	β=40	β =42.7	β=30.74	β=64	β =19.41	β=33.3	β=33.2	β=40
	γ = 25	γ = 25	δ=132	γ = 27.05	γ 2 = 119			γ = 25	γ = 24.24	δ=132
	δ=29.3	δ=29.35	€ = 131	δ1=23.64	€ 1 = 137			δ=29.3	δ=29.3	€ = 131
	€ = 42.2	€ = 42.2	ζ=130	δ2=23.77				€ = 42.2	€ = 42.2	ζ=130

Table S1. ¹H and ¹³C NMR assignment of K11 peptide 1 mM in 10 mM phosphate buffer (10% D₂O), pH 6.6, 278K