Supporting Information

Solution and solid-state NMR structural investigations of the antimicrobial designer peptide GL13K in membranes

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Table S1. Resonance assignments of ^{1}H chemical shifts of *GLK13* at *pH 5* using solution NMR experiments.

Residue	NH (ppm)	CαH (ppm)	CβH (ppm)	Others (ppm)
G1	NA	NA		NA
K2	7.940	4.069	1.803	γ-CH_2 1.321
				δ-CH_2 1.642
				ε-CH_2 2.855
				ε-NH_3^+
I3	7.936	3.949	1.828	γ1-CH_2 1.671
				γ2-CH_3 1.593
				δ-CH_3 0.909
I4	8.732	3.788	1.974	γ1-CH_2 1.671
				γ2-CH_3 1.593
				δ-CH_3 0.909
K5	7.748	4.163	1.832	γ-CH_2 1.408
				δ-CH_2 1.651
				ε-CH_2 2.895
L6	8.342	4.043	1.714	γ-CH 1.506
				δ-CH_3 0.854
K7	8.458	3.801	1.857	γ-CH_2 1.314
				δ-CH_2 1.701
				ε-CH_2 2.820
A8	NA	NA	NA	
S9	7.916	4.227	3.796	
L10	7.637	4.114	1.877	γ-CH 1.561
				δ-CH_3 0.879

K11	7.772	3.991	1.831	γ-CH_2 1.495
				δ-CH_2 1.617
				ε-CH_2 2.908
L12	7.563	4.078	1.808	γ-CH 1.561
				δ-CH_3 0.864
I13	8.094	4.014	1.794	γ1-CH_2 1.671
				γ2-CH_3 1.259
				δ-CH_3 0.832

Table S2 . Statistics for the 20 best NMR structures.

Parameter	Value
Distance and Angle Restraints	
Total NOEs Intraresidual Interresidual	151 70 81
Total restraints per residue	12.6
Statistics for Calculated Structures	
R.M.S.D. (Å) Backbone All Heavy Atoms	 0.29 ± 0.13 1.36 ± 0.40

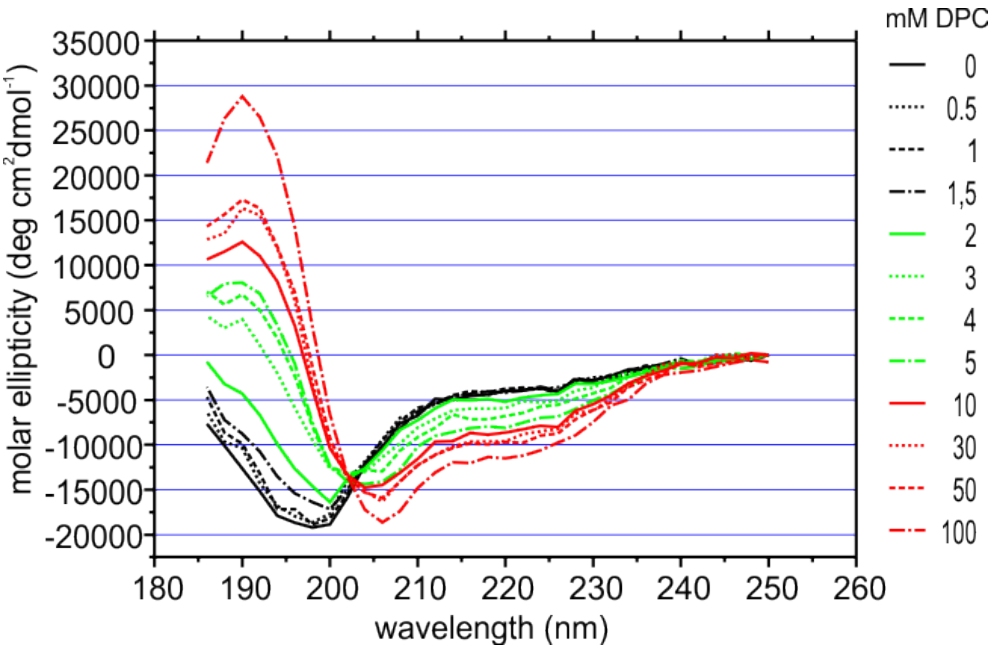

Figure S1: CD spectroscopic titration of 60µM GL13K with DPC in10mM phosphate buffer, pH 5. Line fitting analysis with CD Pro (data set 9) is indicative of about 50%helix content in the presence of 100 mM DPC in reasonable agreement with the NMR structure. The presence of an isosbestic point shows that the interaction of GL13K with DPC is governed by a two-state equilibrium involving random coil and helical conformations.