NMR Structure of Pardaxin, a Pore-Forming Antimicrobial Peptide, in Lipopolysaccharide Micelles: Mechanism of Outer Membrane Permeabilization

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Figure S1

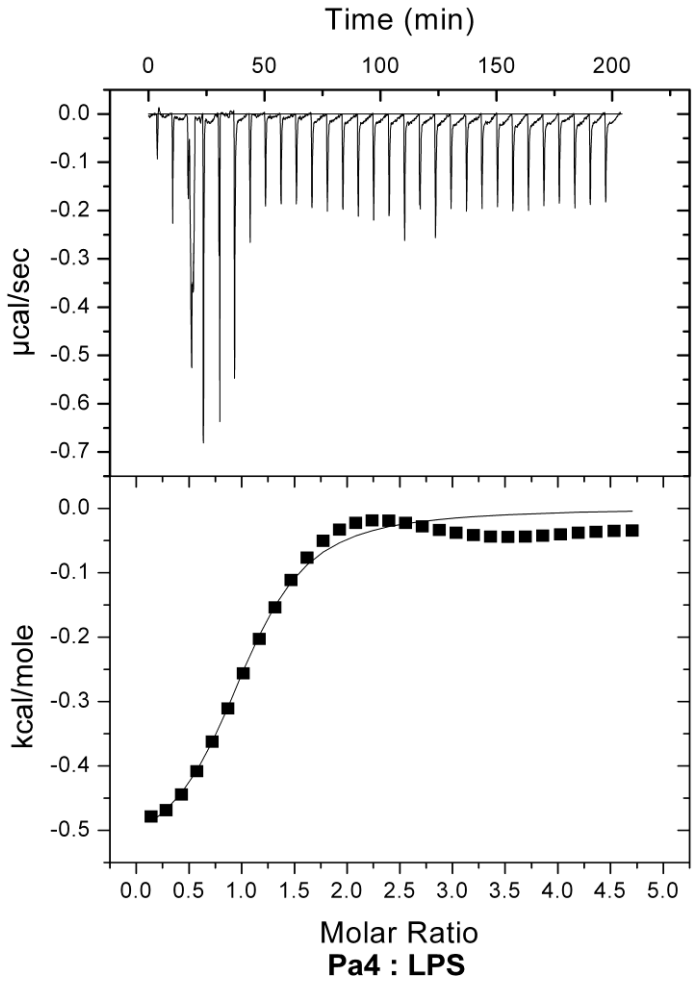

Figure S1: Calorimetric trace of 1 mM Pa4 titrated into 0.05 mM *E. coli* lipopolysaccharide 0111:B4 in 10 mM sodium phosphate, pH 6.2 is shown at 313 K. The upper panel shows the titrated peaks plotted as power (µcal s^{-1}) against time (min). The lower panel shows the corresponding integrated heats of the binding

Figure S2

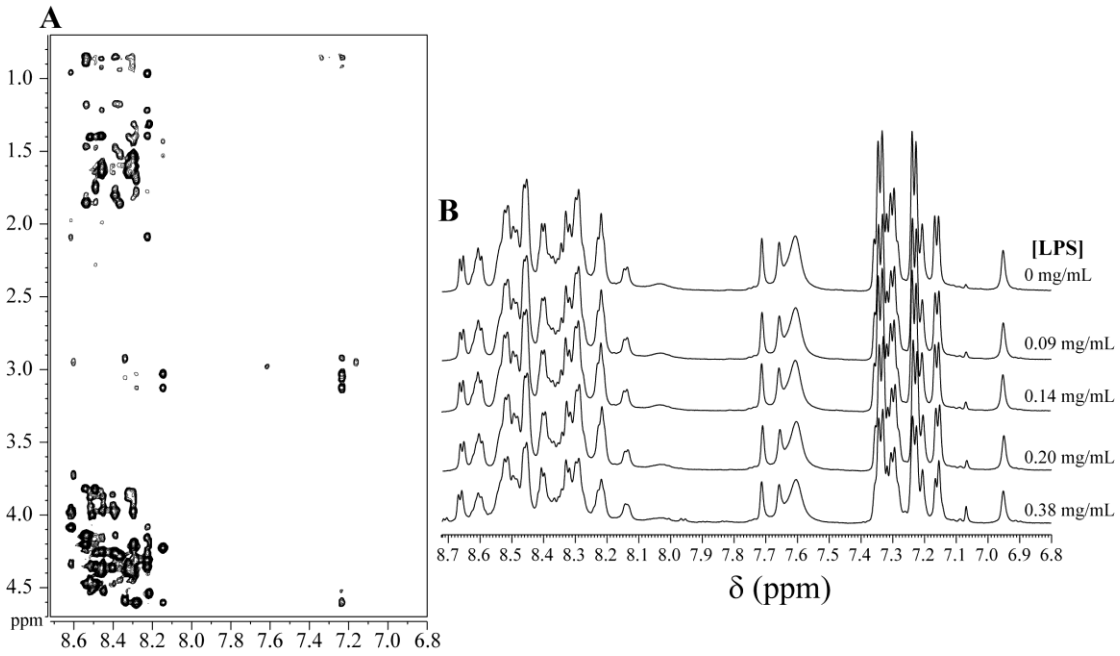

Figure S2: (panel A) Two-dimensional ^{1}H-^{1}H NOESY spectrum of Pa4 in free solution showing NOE connectivities from low field shifted amide/aromatic 1H resonances with aliphatic ^{1}H resonances. (panel B) The low field region of one-dimensional ^{1}H NMR spectra of Pa4 in the presence of different concentrations (shown in right side) of LPS. The experiments were performed at 600 MHz and at 288 K.

Table S1

^{1}H Chemical shifts (in ppm) of the amino acid residues of Pa4 (90% H_20, 10% D_2O), pH 4.5 at 288K. Chemical shifts were referenced to DSS.

Residue	H_N	H_α	$H_{\beta1}$, $H_{\beta2}$	H_γ	H_δ	Others
G1	-	3.728				
F2	8.600	4.598	2.955			2,6H: 7.234 3,5H: 7.334 4H: 7.300
F3	8.337	4.545	3.061, 2.929			2,6H: 7.234 3,5H: 7.334 4H: 7.300
A4	8.216	4.204	1.318			
L5	8.296	4.288	1.604		0.924	
I6	8.364	4.454	1.865	1.183, 0.918	0.860	
P7	-	-	2.285	2.016, 1.971	3.712	
K8	8.491	4.269	1.755	1.479		$C^{\varepsilon}H_2$: 2.996 $N^{\varepsilon}H_3^+$: 7.611
I9	8.388	4.146	1.813	1.171	0.858	
I10	8.538	4.207	1.865	1.472, 1.186	0.900	
S11	8.542	4.476	3.829			
S12	8.400	4.479	3.869			
P13	-	-	2.259	2.016, 1.843	3.776	
L14	8.300	4.234	1.536		0.859	
F15	8.145	4.608	3.132, 3.041			2,6H: 7.237 3,5H: 7.341 4H: 7.305
K16	8.282	4.317	1.782	1.390	1.430	$C^{\varepsilon}H_2$: 2.981 $N^{\varepsilon}H_3^+$: 7.611
T17	8.224	8.258	4.162	1.222		
L18	8.457	4.364	1.612		0.867, 0.929	
L19	8.299	4.370	1.651		0.866	
S20	8.403	4.471	3.933			
A21	8.459	4.369	1.398			
V22	8.224	4.088	2.093	0.961		
G23	8.615	3.983				
S24	8.299	4.457	3.857			
A25	8.517	4.351	1.406			
L26	8.321	1.648			0.933	
S27	8.465	4.512	3.882			
S28	8.517	4.533	3.883			
S29	8.491	4.263	3.832			
G30	8.508	4.003				
G31	8.397	3.971				
Q32	8.457	4.400	1.999	2.356		
E33	8.301	4.403	2.139	2.366		