

Supporting Information for

Structure of a synthetic fragment of the LALF protein when bound to lipopolysaccharide

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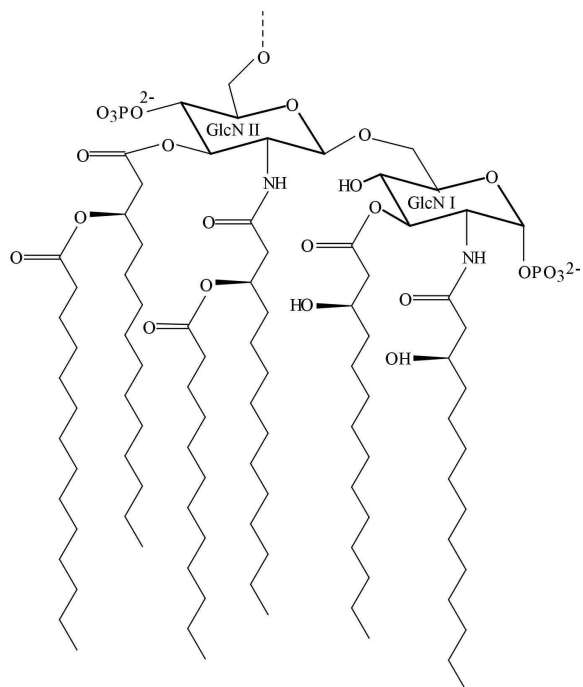
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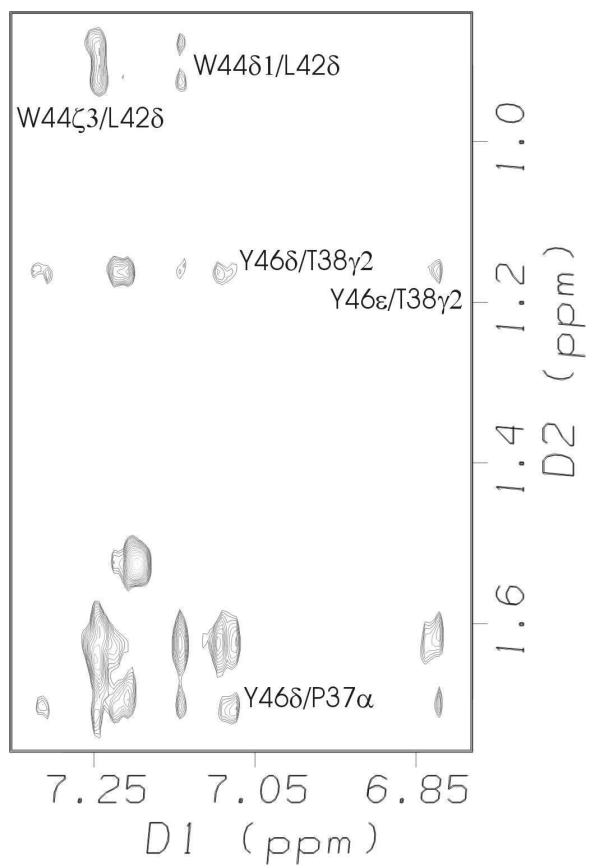
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¹H resonance assignment of LALF-14 (with numbering of residues relative to LALF).

Residue	HN	α	β	others
Gly34	-	3.88		
Cys35	-	4.82	3.17/3.05	
Lys36	8.86	4.70	1.85	γ 1.49, δ 1.73, ϵ 3.02
Pro37	8.77	4.43	2.09/1.70	γ 1.99/1.95, δ 3.86/3.67
Thr38	-	4.32	4.14	γ_2 1.16
Phe39	8.26	4.70	3.14/2.98	δ 7.32, ϵ 7.22
Arg40	8.33	4.17	1.82/1.70	γ 1.53, δ 3.15, ϵ 7.21
Arg41	8.00	4.05	1.92	γ 1.63, δ 3.18, ϵ 7.24
Leu42	8.17	4.36	1.62/1.44	γ 1.62, δ 0.93/0.89
Lys43	8.78	4.26	1.70	γ 1.39, δ 1.66, ϵ 2.95
Trp44	8.53	4.68	3.18	δ_1 7.15, ϵ_1 10.16, ζ_2 7.59, η_2 7.12, ζ_2 7.25, ϵ_3 7.51
Lys45	8.17	4.22	1.62/1.55	γ 1.16, δ 1.60, ϵ 2.92
Tyr46	8.17	4.51	2.97/2.89	δ 7.08, ϵ 6.83
Lys47	8.07	4.33	1.81/1.71	γ 1.34, δ 1.64, ϵ 2.95
Cys48	8.31	4.77	3.26/3.00	
Gly49	8.57	3.80		



Chemical structure of a typical lipid A *E. coli*. The attachment site of the first KDO residue of LPS at the 6-GlcN II oxygen atom is marked with a broken line.



Part of the exchange-transferred NOESY spectrum of LALF-14 (1 mM in 90% H₂O - 10% D₂O at pH 4.5 and 25°C) in mixture with LPS (approx. 10:1 w/w ratio) with a mixing time of 120 ms.