Characterization of Isomeric Lipid A Species from *Pseudomonas aeruginosa* PAO1 by Non-Aqueous Capillary Electrophoresis with Positive and Negative Ion Electrospray Tandem Mass Spectrometry

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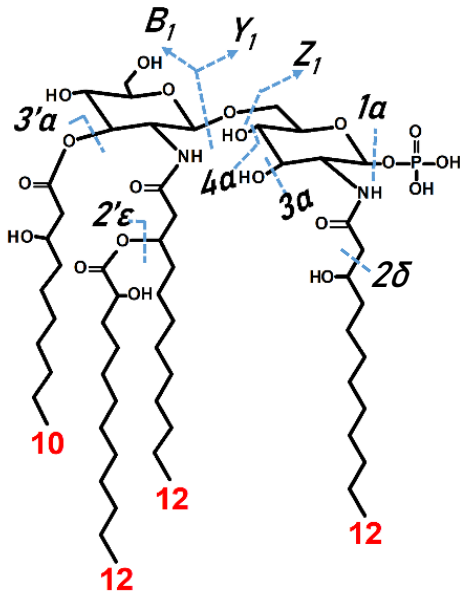

Figure S1 Proposed structure of compound **3***, the minor co-migrating tetra-acylated isomer having a molecular mass of 1184.73 Da. Fragmentation sites are indicated for both ESI polarity modes.

Table S1 Lipid A structures identified from the isolate of strain *P. aeruginosa* PAO1 by NACE–ESI-QTOF MS/MS analysis. Capillary dimensions: 55 cm × 50 μm, applied voltage: 30 kV (reversed CE polarity, detection at the anodic end), pressure assistance: from 0 min: 5 mbar, from 25 min: 30 mbar. BGE: MeOH:$CHCl_3$ 50:50 (v/v) with Et_3N:AcOH 0.72:0.24 (v/v).

t_m (min)	$m_{calc.}$ (Da)	Position on the diglucosamine backbone						reported by
		C4'	C3'	C2'	C3	C2	C1	Buré et al. (2021)
25.91	**1184.73**	H	H	C12:0(3-OH)	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	P	no
26.25	**1184.73**	H	H	C12:0(3-O(C12:0(2-OH)))	C10:0(3-OH)	C12:0(3-OH)	P	no
26.68	**1212.76**	H	H	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-O(C12:0(2-OH)))	P	no
26.89	**1196.77**	H	H	C12:0(3-O(C12:0))	H	C12:0(3-O(C12:0(2-OH)))	P	no
27.02	**1184.73**	H	C10:0(3-OH)	C12:0(3-OH)	H	C12:0(3-O(C12:0(2-OH)))	P	no
27.02	**1184.73**	H	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-OH)	P	no
27.10	**1382.89**	H	H	C12:0(3-O(C12:0(2-OH)))	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	P	no
27.53	**1366.90**	H	H	C12:0(3-O(C12:0))	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	P	no
28.08	**1382.89**	H	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-O(C12:0(2-OH)))	P	no
28.42	**1366.90**	H	C10:0(3-OH)	C12:0(3-O(C12:0))	H	C12:0(3-O(C12:0(2-OH)))	P	no
28.51	**1553.02**	H	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	P	no
29.01	**1537.03**	H	C10:0(3-OH)	C12:0(3-O(C12:0))	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	P	no
29.52	**1184.73**	P	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-OH)	H	yes
30.03	**1184.73**	P	C10:0(3-OH)	C12:0(3-OH)	H	C12:0(3-O(C12:0(2-OH)))	H	yes
30.03	**1382.89**	P	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-O(C12:0(2-OH)))	H	yes
30.16	**1553.02**	P	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	H	yes
30.37	**1366.90**	P	C10:0(3-OH)	C12:0(3-O(C12:0))	H	C12:0(3-O(C12:0(2-OH)))	H	yes
30.50	**1537.03**	P	C10:0(3-OH)	C12:0(3-O(C12:0))	C10:0(3-OH)	C12:0(3-O(C12:0(2-OH)))	H	yes
30.59	**1212.76**	P	H	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-O(C12:0(2-OH)))	H	yes
31.02	**1196.77**	P	H	C12:0(3-O(C12:0))	H	C12:0(3-O(C12:0(2-OH)))	H	no
31.02	**1196.77**	P	H	C12:0(3-O(C12:0(2-OH)))	H	C12:0(3-O(C12:0))	H	no

t_m: migration time; $m_{calc.}$: theoretical molecular mass of lipid A species; **P**: phosphate group.

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