

Conformation of the hexasaccharide repeating subunit from the *Vibrio cholerae* O139 capsular polysaccharide

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Supporting Information.

Characterization of the hexasaccharide isolated from the *V. cholerae* O139 capsular polysaccharide by digestion with bacteriophage polysaccharide lyase.

Fig. S-1 shows the 500 MHz ^1H NMR spectrum of the hexasaccharide recorded at room temperature. The ^1H and ^{13}C assignments summarized in Table S-1 are consistent with those reported by Linnerborg et al (2001) indicating that we have isolated the same product as that which they described. The paper of Linnerborg et al., (2001) reports FAB mass spectra for the hexasaccharide product of bacteriophage digestion as well as other GCMS and Maldi spectra characterizing the 12 residue oligosaccharide containing two repeating units from the polysaccharide which is isolated by incomplete lyase digestion of the O139 polysaccharide.

Linnerborg, M., Weintraub, A., Albert, M.J. and Widmalm, G (2001) *Carbohydr. Res.* 333, 263-269.

Table S-1 Assignment data for the hexasaccharide at 27° C

Position	Proton	Carbon	Position	Proton	Carbon
QuiNAc			Gal		
A1	4.60	100.3	E1	4.71	101.7
A2	3.75	54.7	E2	3.624	77.0
A3	3.78	79.0	E3	3.90	73.3
A4	3.476	77.0	E4	4.58	77.3
A5	3.480	72.6	E5	3.62	68.2
A6,CH3	1.31	17.1	E6	4.34	69.6
ANAc	2.056	23.1	E6'	4.41	69.6
α -GlcNAc			Col ⁴		
Ba1	5.03	91.7	F1	4.76	98.6
Ba2	3.92	55.2	F2	3.975	64.3
Ba3	4.21	73.9	F3a	2.064	33.5
Ba4	3.70	72.8	F4	4.20	69.6
Ba5	4.02	70.6	F5	4.71	66.9
Ba6	3.93	67.0	F6,CH3	1.168	16.4
Ba6'	4.07	67.0			
BaNAc	2.072	22.8			
Δ 4,5 GalA			β -GlcNAc (minor)		
C1	5.73	100.0	Bb1	4.59	96.5
C2	3.75	70.9	Bb2	3.79	57.4
C3	4.33	66.0	Bb3	4.02	76.2
C4,C=C	5.90	110.6	Bb4	3.67	72.6
			Bb5	3.57	75.0
			Bb6	3.88	66.9
			Bb6'	4.16	66.9
Col ²					
D1	5.00	100.2			
D2	3.971	64.3			
D3a	1.813	33.6			
D3e	1.896	33.6			
D4	3.76	69.6			
D5	4.27	67.0			
D6,CH3	1.182	16.4			

D3a=D3axial; D3e=D3equatorial

