

Supplementary Table 2 ^1H and ^{13}C NMR chemical shifts of O-acetylated and non-O-acetylated monosaccharide residues in *S. flexneri* O-polysaccharides

Sugar unit	Monosaccharide						O-Acetyl group	
	H-3	C-3	H-4	C-4	H-6a, 6b	C-6	H-2	C-2
Sf301 oacD								
Rhap ^{III} 3Ac	5.08	73.8					2.21	21.8
Rhap ^{III} 4Ac			4.80	75.4			2.16	21.7
Glc p NAc					3.77, 3.91	61.9		
Sf301 oacD_pSQZ6								
Rhap ^{III} 3Ac	5.08	73.9					2.21	21.8
Rhap ^{III} 4Ac			4.79	75.4			2.16	21.7
Glc p NAc6Ac					4.32, 4.41	64.5	2.14	21.5
51571 (1a)								
Rhap ^{III} 3Ac	5.08	74.2					2.21	21.9
Rhap ^{III} 4Ac			4.82	75.6			2.17	21.8
Glc p NAc					3.84, 3.84	62.6		
51571_pSQZ6								
Rhap ^{III} 3Ac	5.07	73.6					2.20	21.8
Rhap ^{III} 4Ac			4.80	75.3			2.15	21.7
Glc p NAc6Ac					4.32, 4.42	64.1	2.14	21.6
51577 (4b)								
Rhap ^{III}	3.86	71.2	3.30	73.5				
Glc p NAc					3.78, 3.98	67.0 ^a		
51577_pSQZ6								
Rhap ^{III}	3.86	70.9	3.30	73.5				
Glc p NAc6Ac					4.30, 4.41	64.3	21.4	21.5

^aThe signal is shifted downfield owing to glucosylation at position 6.