



Title	Metabolic Mechanism of Mannan in a Ruminant Bacterium, <i>Ruminococcus albus</i> , Involving Two Mannoside Phosphorylases and Cellobiose 2-Epimerase : Discovery of a New Carbohydrate Phosphorylase, β -1,4-Mannooligosaccharide Phosphorylase
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Table S1. Chemical shifts of products of synthetic reactions of rRaMP1 and rRaMP2 in the ¹H- and ¹³C- NMR spectra.

(a) Man-Glc

		δ_C (ppm)	δ_H (ppm)		J (H, H)
Man	1	102.87 ^{*a}	4.75 ^{*b}	d	0.9
	2	73.36	4.07	m	
	3	75.62	3.65	dd	1.5, 3.1
	4	69.45	3.58	m	
	5	79.23	3.42	ddd	2.4, 6.8, 9.5
	6	63.74	3.95	dd	2.3, 12.2
α -Glc (41%)			3.75	m	
	1	94.65	5.23	d	3.9
	2	73.93	3.59	m	
	3	74.12	3.88	dd	2.7, 10.8
	4	81.64 ^{*b}	3.67 ^{*a}	m	
	5	72.75	3.93	m	
β -Glc (59%)	6	62.95	3.81	m	
			3.77	m	
	1	98.59	4.67	d	8.1
	2	76.59	3.29	dd	8.0, 9.4
	3	77.04	3.67	m	
	4	81.53 ^{*b}	3.68 ^{*a}	m	
5	77.43	3.59	m		
6	63.06	3.73	dd	2.6, 12.3	
			3.86	m	

*HMBC cross peaks were observed.

(b) 4-*O*- β -D-mannosyl-D-xylose

		δ_C (ppm)	δ_H (ppm)		J (H, H)
Man	1	101.17 ^{*a}	4.79 ^{*b}	s	
	2	73.59	3.98	dd	3.1, 0.9
	3	75.68	3.66	m	
	4	69.57	3.57	m	
	5	79.14	3.42	m	
	6	63.85	3.74	dd	12.2, 2.3
α -Xyl (36%)			3.93	dd	12.3, 6.5
	1	94.78	5.19	d	3.7
	2	73.99	3.59	m	
	3	73.91	3.81	m	
	4	79.22 ^{*b}	3.84 ^{*a}	m	
	5	61.53	3.82	m	
β -Xyl (64%)			3.73	m	
	1	99.29	4.59	d	7.9
	2	76.59	3.27	dd	9.3, 7.9
	3	76.87	3.60	m	
	4	79.14 ^{*b}	3.88 ^{*a}	m	
	5	65.76	4.06	dd	11.6, 5.4
			3.37	m	

*HMBC cross peaks were observed.

(c) 4-*O*-β-D-mannosyl-cellobiose

		δ_C (ppm)	δ_H (ppm)	J (H, H)	
Man	1	102.86 ^{*a}	4.75 ^{*b}	s	
	2	73.35	4.06	d	3.1
	3	75.60	3.65	m	
	4	69.45	3.59	m	
	5	79.21	3.42	ddd	1.8, 6.8, 9.4
	6	63.74	3.94	m	
Glc	1	105.17 ^{*c}	4.54 ^{*d}	d	7.8
	2	75.62	3.37	m	
	3	76.81	3.69	m	
	4	81.32 ^{*b}	3.69 ^{*a}	m	
	5	77.44	3.61	m	
	6	62.90	3.74	m	
α -Glc (39%)	1	94.63	5.23	d	3.9
	2	74.04	3.83	m	
	3	74.10	3.58	m	
	4	81.44 ^{*d}	3.67 ^{*c}	m	
	5	72.93	3.96	m	
	6	62.69	3.87	m	
β -Glc (61%)	1	98.56	4.66	d	7.8
	2	76.71	3.28	dd	8.1, 9.2
	3	77.05	3.64	m	
	4	81.28 ^{*d}	3.67 ^{*c}	m	
	5	77.61	3.61	m	
	6	62.82	3.80	m	
			3.95	m	

*HMBC cross peaks are observed.

(d) 4-*O*- β -D-mannosyl-*N,N'*-diacetylchitobiose

		δ_C (ppm)	δ_H (ppm)		<i>J</i> (H, H)
Man	1	102.88	4.77 ^{*a}	s	
	2	73.30	4.07	d	3.3
	3	75.57	3.78	m	
	4	69.42	3.58	m	
	5	79.22	3.43	m	
	6	63.73	3.72	m	
GlcNAc			3.93	dd	2.2, 12.3
	1	104.19 ^{*b}	4.62 ^{*b}	d	7.9
	2	57.86	3.77	m	
	C=O	177.38			
	CH ₃	24.91	2.07	s	
	3	74.79	3.77	m	
	4	81.46 ^{*a}	3.76	m	
	5	77.39	3.62	m	
α -GlcNAc (77%)	6	62.87	3.69	m	
			3.77	m	
	1	93.23	5.20	d	2.5
	2	56.44	3.89	m	
	C=O	177.27			
	CH ₃	24.68	2.05	s	
	3	72.05	3.89	m	
	4	82.51 ^{*b}	3.64 ^{*b}	m	
β -GlcNAc (23%)	5	75.29	3.67	m	
	6	62.81	3.81	m	
			3.88	m	
	1	97.62	4.70	d	8.2
	2	58.91	3.69	m	
	C=O				
	CH ₃				
	3	72.80	3.89	m	
4	82.06	3.65 ^{*b}	m		
5	77.39	3.53	m		
6	62.93	3.66	m		
			3.86	m	

*HMBC cross peaks are observed. Cross peaks between C1 of mannosyl residue and H4 of GlcNAc and between H1 of internal GlcNAc and C4 of β -GlcNAc were not detected.