Isolation, chemical characterization, and immunomodulatory activity of naturally acetylated hemicelluloses from bamboo shavings

Supplementary materials

Table S1 ^{1}H NMR chemical shifts (relative to an internal H_2O, δ_H=4.70 ppm) of constituent monosaccharide residues in BSH-1 and BSH-2

Residue[a]	Chemical shifts (ppm)								
	H-1	H-2	H-3	H-4	H-5ax	H-5eq	CH_3(Ac)	O-CH_3	COOH
BSH-1									
β-X_{red}	4.56	3.20	3.63	n.d.	n.d.	4.09	--	--	--
X_{int}	4.42	3.24	3.50	3.72	3.41	4.05	--	--	--
X'_{int}	4.36	3.14	3.47	3.69	3.32	4.00	--	--	--
X_{term}	4.39	n.d.	n.d.	3.63	n.d.	n.d.	--	--	--
X_{A3}	4.52	3.54	3.66	n.d.	n.d.	n.d.	--	--	--
X_{Ac2}	4.63	4.63	3.75	3.86	n.d.	n.d.	2.05	--	--
X_{Ac3}	4.50	3.51	4.92	3.89	3.41	n.d.	2.09	--	--
A_3	5.32	4.34	n.d.	n.d.	3.69	3.82	--	--	--
BSH-2									
β-X_{red}	4.53	3.16	3.61	n.d	n.d	4.05	--	--	--
X_{int}	4.39	3.20	3.46	3.70	3.37	4.00	--	--	--
X'_{int}	4.34	3.10	3.43	3.68	3.28	3.96	--	--	--
X_{term}	4.31	n.d.	n.d.	3.61	3.33	n.d.	--	--	--
$X_{MeGlcA2}$	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	--	--	--
X_{A3}	4.57	3.51	3.63	n.d.	n.d.	n.d.	--	--	--
X_{Ac2}	n.d.	4.59	3.71	3.83	n.d.	n.d.	2.02	--	--
X_{Ac3}	4.48	3.38	4.89	3.87	3.38	n.d.	2.06	--	--
X_{Ac23}	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	2.13	--	--
A_3	5.32	n.d.	n.d.	n.d.	3.66	3.78	--	--	--
$MeGlcA_2$	5.19	3.57	3.81	3.21	4.31	--	--	3.35	n.d.

[a] The following designations are used. H_{ax}, axial proton; H_{eq}, equatorial proton; β-X_{red}, Xyl unit with reducing end; X_{int}(X'_{int}), Xyl internal; X_{term}, Xyl with terminal end; $X_{MeGlcA2}$, MeGlcA 2-*O*-linked Xyl; X_{A3}, Ara 3-*O*-substituted Xyl; X_{Ac2}, 2-*O*-acetylated Xyl; X_{Ac3}, 3-*O*-acetylated Xyl; X_{Ac23}, 2,3-di-*O*-acetylated Xyl; A_3, 3-*O*-linked Ara; $MeGlcA_2$, 2-*O*-linked MeGlcA; n.d., not detected; Xyl, xylose; Ara, arabinose; MeGlcA, 4-*O*-methyl-glucuronic acid

Table S2 ^{13}C NMR chemical shifts (relative to an internal acetone-d_6, δ_C=30.50 ppm) of constituent monosaccharide residues in BSH-1 and BSH-2

Residue[a]	Chemical shifts (ppm)								
	C-1	C-2	C-3	C-4	C-5	CH_3(Ac)	C=O(Ac)	O-CH_3	COOH
BSH-1									
β-X_{red}	97.52	74.98	72.80	n.d.	63.94	--	--		
X_{int}	102.66	73.65	74.63	77.33	63.94	--	--		
X'_{int}	103.63	73.73	74.54	77.13	63.94	--	--		
X_{term}	102.81	73.80	76.59	70.34	66.21	--	--		
X_{A3}	101.81	n.d.	74.91	n.d.	n.d.	--	--		
X_{Ac2}	100.83	74.46	72.47	n.d.	63.94	21.37	173.96		
X_{Ac3}	102.43	71.87	76.20	76.47	63.94	21.60	174.49		
X_{Ac23}	n.d.	72.42	73.93	n.d.	63.94	n.d.	n.d.		
A_3	n.d.	n.d.	n.d.	n.d.	61.44	--	--		
BSH-2									
β-X_{red}	97.46	74.94	72.70	77.86	63.91	--	--	--	--
X_{int}	102.61	73.63	74.58	77.28	63.91	--	--	--	--
X'_{int}	103.60	73.53	74.49	77.07	63.91	--	--	--	--
X_{term}	102.76	73.85	n.d.	70.28	66.16	--	--	--	--
X_{A3}	101.91	n.d.	74.85	n.d.	n.d.	--	--	--	--
X_{GlcA2}	102.94	75.61	n.d.	n.d.	n.d.	--	--	--	--
X_{Ac2}	100.79	74.41	72.42	n.d.	63.91	21.36	174.07	--	--
X_{Ac3}	102.38	71.83	76.17	76.47	63.91	21.59	174.60	--	--
X_{Ac23}	n.d.	72.34	73.85	n.d.	63.91	22.03	174.75	--	--
A_3	n.d.	82.26	81.63	n.d.	61.38	--	--	--	--
$MeGlcA_2$	98.74	n.d.	73.24	83.16	n.d.	--	--	61.00	176.95

[a] The following designations are used: β-X_{red}, Xyl with reducing end; X_{int}(X'_{int}), Xyl internal; X_{term}, Xyl with terminal end; $X_{MeGlcA2}$, MeGlcA 2-*O*-linked Xyl; X_{A3}, Ara 3-*O*-substituted Xyl; X_{Ac2}, 2-*O*-acetylated Xyl; X_{Ac3}, 3-*O*-acetylated Xyl; X_{Ac23}, 2,3-di-*O*-acetylated Xyl; A_3, 3-*O*-linked Ara; $MeGlcA_2$, 2-*O*-linked MeGlcA; n.d., not detected; Xyl, xylose; Ara, arabinose; MeGlcA, 4-*O*-methyl-glucuronic acid