Supplementary data

Diluted aqueous ionic liquid assists acidic oxidative hydrolysis of water-soluble recalcitrant polysaccharide xanthan through structural deterioration

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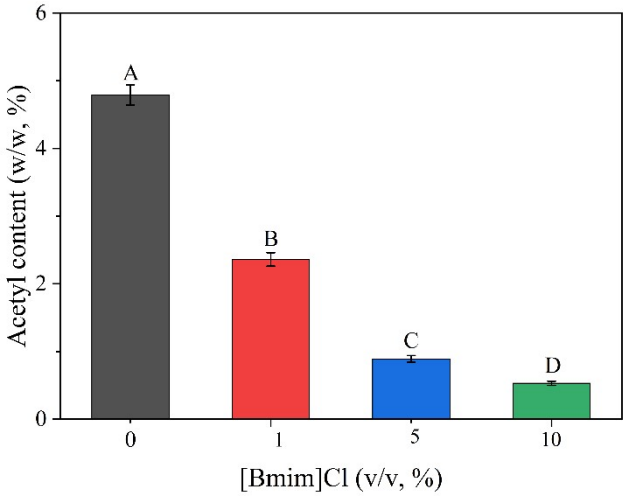

Fig. S1. Acetyl content analysis of different XG samples. XG samples were washed with ethanol to remove [Bmim]Cl. Acetyl content of different XG samples were characterized by measuring the absorbance at 540 nm of complexes formed by the reaction of acetyl groups, hydroxylamine, and $FeCl_3$. Different letters represent significant differences ($P < 0.05$).

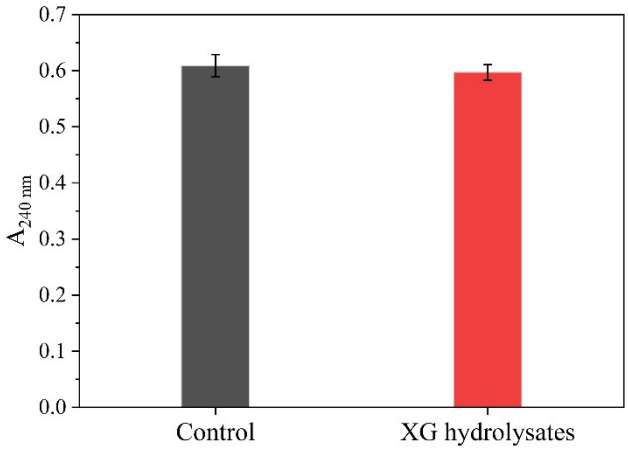

Fig. S2. The content of H_2O_2 in different XG hydrolysates. XG hydrolysates and control sample were prepared in a system containing 0.4 M HCl, 0.75% (w/v) H_2O_2, and with or without 1% (v/v) [Bmim]Cl at 80 °C for 4 days.

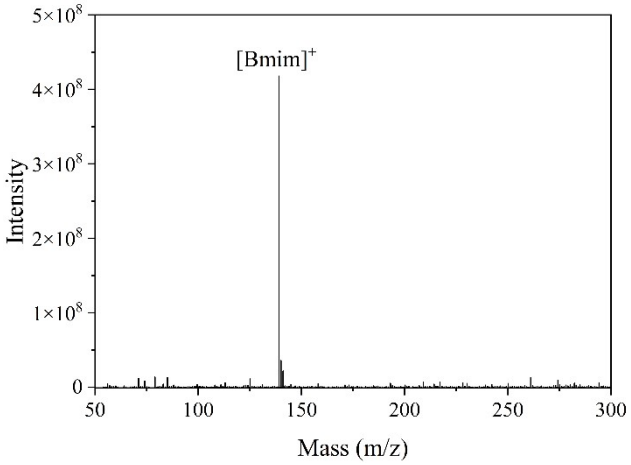

Fig. S3. ESI-MS analysis of recovered [Bmim]Cl.

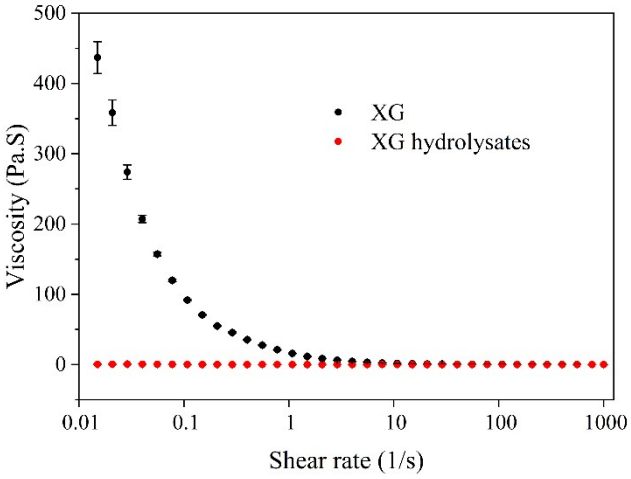

Fig. S4. Viscosity analysis of native XG and its hydrolysates. XG hydrolysates were prepared in the system containing 0.4 M HCl, 0.75% (w/v) H_2O_2 and 1% (v/v) [Bmim]Cl at 80 ^oC for 4 days.

Table S1 Mass balance of XG hydrolysis process

Component	Mass (g)	Yield (%)
Recovered XG hydrolysate	1.23	24.64
Glucose	0.69	13.79
Mannose	0.89	17.80
Glucuronic acid	1.05	20.98
Trisaccharide	0.22	4.34
Tetrasaccharide	0.071	1.41
Furfural	0.016	0.31
Acetic acid	0.0083	0.17
Solid residues	0.33	6.60

Yield = Products mass/native XG mass ×100%

Table S2 2D NMR HSQC data of XG hydrolysates

δ(ppm)		Assignment
^{1}H	^{13}C	
3.1-4.3	65-81	C2/H2, C3/H3, C4/H4 and C5/H5 (COOH) of basic units (glucose, glucuronic acid and mannose)
3.5-4.1	60.5	C6/H6 of glucose and mannose
4.5	96.0	C1/H1 and C6/H6 of glucuronic acid
4.9	93.5	C1/H1 of mannose
5.1	91.8	C1/H1 of glucose

Table S3 Band assignments in FTIR spectra of XG hydrolysates

Band (cm^{-1})	Assignment
3417-3421	O-H stretching
2926	C−H of methyl group
1728	-C=O of acetyl group
1626-1627	-C=O of pyruvate group
1408-1417	-C-H of methyl group
1386-1384	-C-H of methylene group
1258	C-O of carbonyl group
1048-1050	C-O-C-O-C stretching
793	-C-H of methyl group
600	O-C=O stretching

Table S4 MALDI-TOF MS results for XG hydrolysates.

Code	MALDI-TOF Mass (m/z)		Structure	DP	Code	MALDI-TOF Mass (m/z)		Structure	DP
XGOS1	527.08	$[M+Na]^+$	Hex_3	3	XGOS19#	2604.11	$[M+Na]^+$	$Ac_3Hex_{12}HexA_2Pyr_2$	14
XGOS2	541.06	$[M+Na]^+$	Hex_2HexA_1	3			$[M+H]^+$	$Ac_1Hex_{12}HexA_3Pyr_1$	15
XGOS3	689.13	$[M+Na]^+$	Hex_4	4			$[M+H]^+$	$Ac_3Hex_{13}HexA_2$	15
XGOS4	703.10	$[M+Na]^+$	Hex_3HexA_1	4	XGOS20	2637.72	$[M+H]^+$	$Ac_4Hex_{11}HexA_3Pyr_2$	14
XGOS5	851.17	$[M+Na]^+$	Hex_5	5	XGOS21#	2701.97	$[M+H]^+$	$Hex_{12}HexA_3Pyr_3$	15
XGOS6	865.12	$[M+Na]^+$	Hex_4HexA_1	5			$[M+H]^+$	$Ac_5Hex_{12}HexA_3$	15
XGOS7	1013.20	$[M+Na]^+$	Hex_6	6			$[M+H]^+$	$Ac_2Hex_{13}HexA_2Pyr_2$	15
XGOS8	1027.13	$[M+Na]^+$	Hex_5HexA_1	6			$[M+H]^+$	$Ac_4Hex_{14}HexA_1Pyr_1$	15
XGOS9	1175.20	$[M+Na]^+$	Hex_7	7			$[M+H]^+$	Ac_6Hex_{15}	15
XGOS10	1247.14	$[M+K]^+$	$Ac_1Hex_6HexA_1$	7	XGOS22#	2758.18	$[M+H]^+$	$Ac_3Hex_{12}HexA_3Pyr_2$	15
XGOS11	1409.18	$[M+K]^+$	$Ac_1Hex_7HexA_1$	8			$[M+H]^+$	$Ac_5Hex_{13}HexA_2Pyr_1$	15
XGOS12	1571.20	$[M+K]^+$	$Ac_1Hex_8HexA_1$	9	XGOS23#	2831.18	$[M+K]^+$	$Hex_{13}HexA_3Pyr_2$	15
XGOS13	1733.21	$[M+K]^+$	$Ac_1Hex_9HexA_1$	10			$[M+K]^+$	$Ac_2Hex_{14}HexA_2Pyr_1$	16
XGOS14	2118.12	$[M+H]^+$	$Ac_3Hex_{10}HexA_2$	12			$[M+K]^+$	$Ac_4Hex_{15}HexA_1$	16
XGOS15	2215.29	$[M+H]^+$	$Ac_2Hex_{10}HexA_2Pyr_2$	12	XGOS24#	2892.55	$[M+H]^+$	$Ac_4Hex_{13}HexA_3Pyr_1$	16
XGOS16#	2423.33	$[M+K]^+$	$Hex_{12}HexA_2Pyr_1$	14			$[M+H]^+$	$Ac_6Hex_{14}HexA_2$	16
		$[M+K]^+$	$Ac_2Hex_{13}HexA_1$	14	XGOS25#	2955.11	$[M+Na]^+$	$Ac_5Hex_{13}HexA_3Pyr_1$	16
XGOS17#	2526.45	$[M+H]^+$	$Ac_3Hex_{11}HexA_3Pyr_1$	14			$[M+H]^+$	$Ac_3Hex_{13}HexA_4$	17
		$[M+H]^+$	$Ac_5Hex_{12}HexA_2$	14			$[M+H]^+$	$Hex_{14}HexA_3Pyr_2$	17
XGOS18#	2540.35	$[M+H]^+$	$Ac_5Hex_{11}HexA_3$	14			$[M+H]^+$	$Ac_2Hex_{15}HexA_2Pyr_1$	17
		$[M+H]^+$	$Ac_2Hex_{12}HexA_2Pyr_2$	14			$[M+H]^+$	$Ac_4Hex_{16}HexA_1$	17
		$[M+H]^+$	$Ac_4Hex_{13}HexA_1Pyr_1$	14					

Ac, acetyl group; Hex, hexose; HexA, glucuronic acid; Pyr, pyruvate group; #indicates different possible conformations for the same m/z ion.