

Supporting Information

A lignin-containing cellulose hydrogel for lignin fractionation

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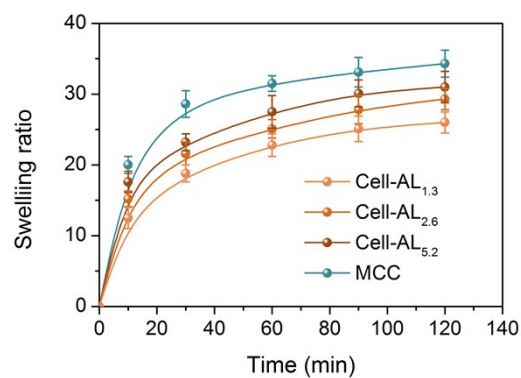


Fig. S1 Swelling behaviours of the hydrogels in distilled water at 25 °C.

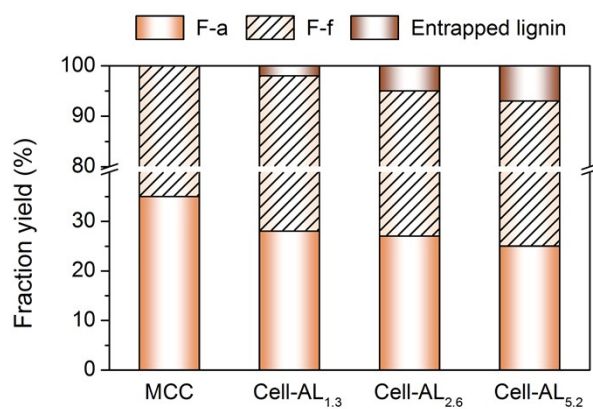


Fig. S2 The fraction yields of F-a, F-f, and entrapped lignin.

Table S1. The molecular weight and content of the hydroxyl and carboxyl groups of AL and lignin fractions.

Label	AL	F-a				F-f			
		MCC	Cell-AL _{1,3}	Cell-AL _{2,6}	Cell-AL _{5,2}	MCC	Cell-AL _{1,3}	Cell-AL _{2,6}	Cell-AL _{5,2}
M_w (g/mol)	1054	998	881	752	499	1059	1097	1180	1220
M_n (g/mol)	737	713	672	592	442	751	819	994	1008
M_w/M_n	1.43	1.40	1.31	1.27	1.13	1.41	1.34	1.25	1.21
Total ^a S	0.65	0.60	0.51	0.50	0.46	0.58	0.46	0.47	0.43
Total G	0.96	0.86	0.74	0.70	0.65	0.85	0.71	0.68	0.6
Nonph ^b S	0.55	0.49	0.42	0.41	0.37	0.50	0.39	0.40	0.37
Nonph G	0.87	0.79	0.64	0.63	0.59	0.77	0.62	0.61	0.55
Nonph H	0.92	0.83	0.66	0.64	0.60	0.79	0.62	0.61	0.57
Total –COOH	1.98	1.96	1.49	1.55	1.60	2.01	1.51	1.64	1.66
Total aliphatic	3.52	2.66	3.55	4.43	5.71	2.70	3.63	4.61	5.79

^a Hydroxyl groups: mmol g⁻¹, ^b Nonph means the noncondensed phenolic –OH.

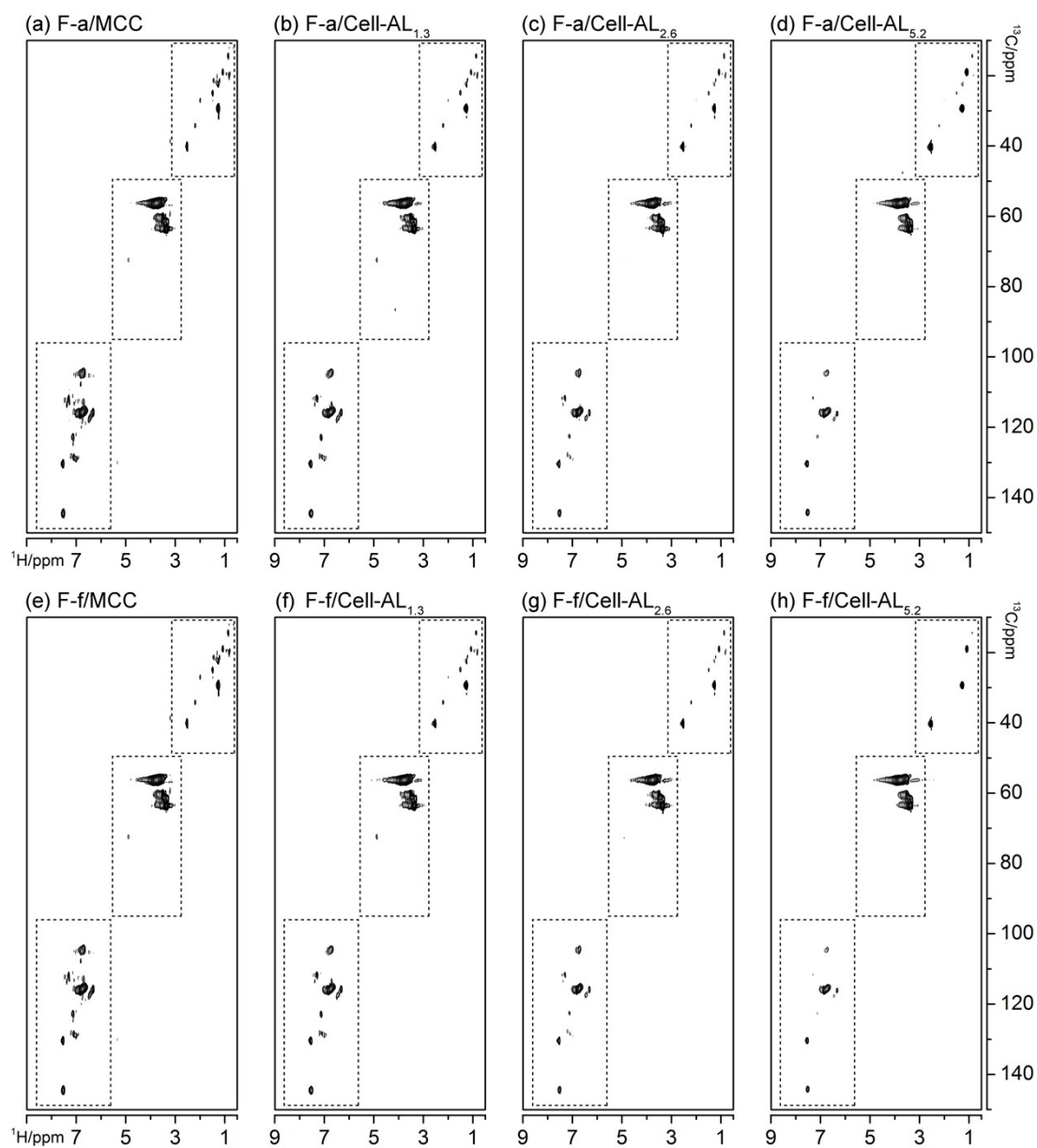


Fig. S3 2D HSQC NMR spectra for the (a-d) filtered and (e-h) adsorbed lignin fractions.

Table S2. Assignment of ^{13}C - ^1H cross-signals in the HSQC spectra of the samples.

Label	$\delta_{\text{C}}/\delta_{\text{H}}$ (ppm)			Assignment
	AL	F-a/MCC	F-a/Cell-AL _{2,6}	
–OCH ₃	56.2/3.75	56.2/3.75	56.2/3.75	C–H in methoxyls
A _{γ}	60.2/3.42 and 3.70	60.4/3.46 and 3.71	60.3/3.48 and 3.74	C _{γ} –H _{γ} in β -O-4' substructures (A)
B _{γ}	62.9/3.70	63.1/3.73	63.2/3.76	C _{γ} –H _{γ} in phenylcoumaran substructures (B)
A _{α}	72.5/4.88	72.5/4.89	72.6/4.89	C _{α} –H _{α} in β -O-4' substructures (A)
S _{2,6}	104.2/6.71	104.2/6.71	104.2/6.71	C _{2,6} –H _{2,6} in syringyl (S)
G ₂	111.0/7.13	111.1/7.13	111.0/7.13	C ₂ –H ₂ in guaiacyl (G)
G ₅ /G ₆	115.7/6.71 and 6.93 118.9/6.82	115.7/6.72 and 6.97 118.5/6.74	115.7/6.72 and 6.92 118.3/6.73	C ₅ –H ₅ and C ₆ –H ₆ in guaiacyl (G)
G' ₂	111.8/7.28 and 7.45	111.8/7.28 and 7.45	111.8/7.28 and 7.45	C ₂ –H ₂ in oxidized guaiacyl (G)
G' ₅	113.2/6.70	113.2/6.70	113.2/6.68	C ₅ –H ₅ in oxidized guaiacyl (G)
FA ₂	113.7/7.38	113.6/7.37	113.6/7.37	C ₂ –H ₂ in ferulates (FA)
H _{3,5}	114.5/6.70	114.6/6.74	114.6/6.73	C _{3,5} –H _{3,5} <i>p</i> -hydroxyphenyl (H)
PCA _{β}	115.5/6.53	115.3/6.54	115.3/6.53	C _{β} –H _{β} in <i>p</i> -counmarates (PCA)
FA ₅	116.1/6.80	116.1/6.82	116.2/6.82	C ₅ –H ₅ in ferulates (FA)
PCA _{3,5}	116.7/6.72	116.7/6.72	116.8/6.72	C _{3,5} –H _{3,5} in <i>p</i> -counmarates (PCA)
FA ₆	122.5/7.13	122.7/7.12	122.5/7.13	C ₆ –H ₆ in ferulates (FA)
H _{2,6}	127.8/7.21	128.0/7.19	127.9/7.19	C _{2,6} –H _{2,6} <i>p</i> -hydroxyphenyl (H)
PCA _{2,6}	130.5/7.53	130.6/7.52	130.6/7.52	C _{2,6} –H _{2,6} in <i>p</i> -counmarates (PCA)
FA _{α} /PCA _{α}	144.5/7.52	144.7/7.52	144.7/7.52	C _{α} –H _{α} in ferulates (FA) and <i>p</i> -counmarates (PCA)

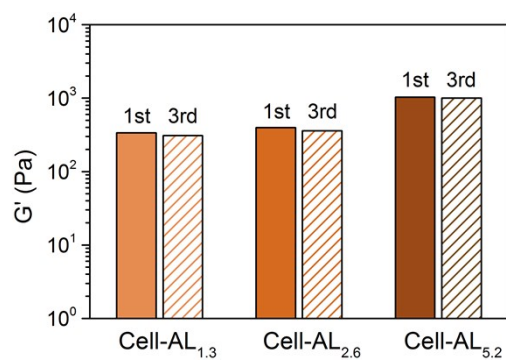


Fig. S4 The storage modulus (G' , under the 1000% strain) of the original samples and after fractionating lignin three times.

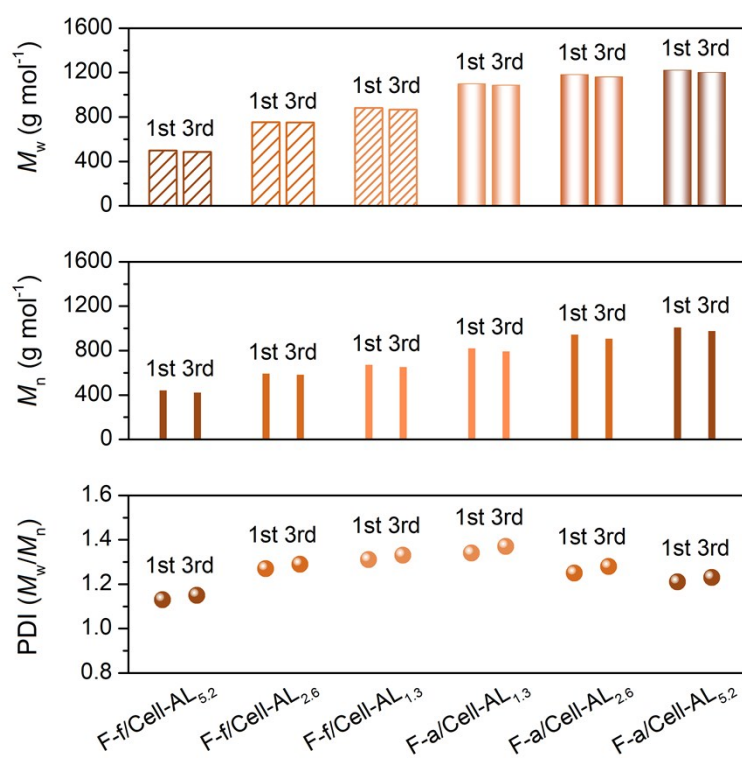


Fig. S5 M_w , M_n and PDI values of lignin fractions after the first and third fractionation.

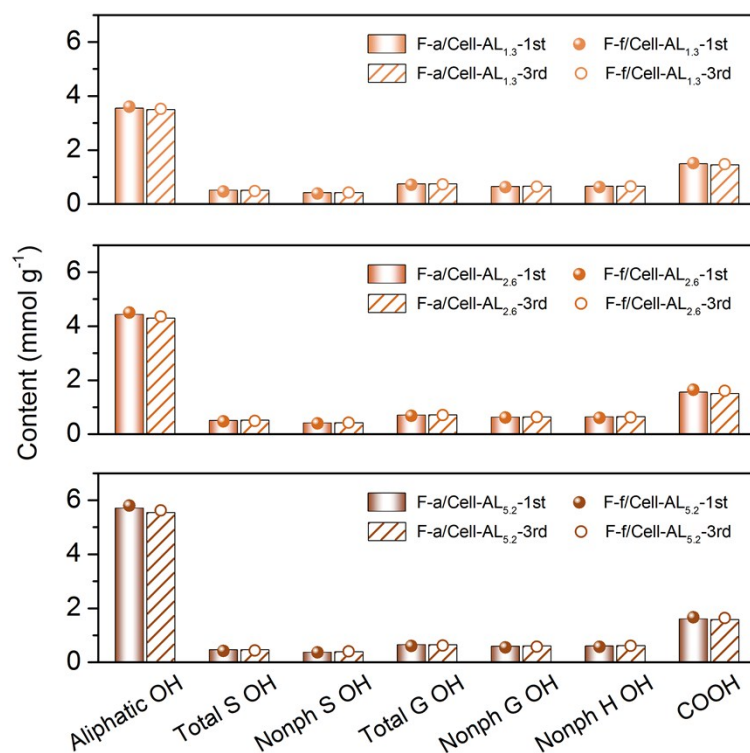


Fig. S6 Content in hydroxyl and carboxyl groups of lignin fractions after the first and third fractionation. Nonph means the noncondensed phenolic hydroxyl groups.