Supporting Information

Dual Effects of lignin derivatives produced by hydrothermal pretreatment on Cellulase Hydrolysis

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Table S1. Chemical components of pseudo-lignin.

Samples	PL-M-1	PL-M-2	PL-M-3	PL-M-4	PL-P-1	PL-P-2	PL-P-3	PL-P-4	PL-W-1	PL-W-2	PL-W-3	PL-W-4
Lignin (%)	2.4	2.9	11.4	14.7	32.2	28.9	24.3	24.0	12.1	9.5	6.6	4.5

Carbohydrates were not detected.

Table S2. Chemical components of lignin-like substances.

Samples	Chemical compositions (%)					
	Lignin	Glucose	Xylose	Galactose	Arabinose	Mannose
LL-M-2	2.7	10.0	14.3	3.0	2.4	31.9
LL-M-3	3.3	12.6	14.2	2.9	1.6	32.7
LL-M-4	14.6	20.2	9.1	1.3	1.1	33.2
LL-P-2	5.9	2.7	40.4	4.0	2.0	4.1
LL-P-3	8.1	4.9	39.8	3.8	1.2	4.9
LL-P-4	9.0	13.6	25.1	0.7	0.9	5.9
LL-W-2	10.3	2.1	26.0	3.5	1.9	1.5
LL-W-3	15.1	2.8	23.0	3.3	1.5	2.2
LL-W-4	20.3	9.2	10.9	0.5	0.7	2.4

Table S3. Molecular weight of pseudo-lignin.

Samples	M_n (g/mol)	M_w (g/mol)	PDI (M_w/M_n)
PL-M-1	622	720	1.16
PL-M-2	718	846	1.18
PL-M-3	702	831	1.18
PL-M-4	770	1009	1.31
PL-P-1	659	781	1.20
PL-P-2	713	860	1.21
PL-P-3	724	871	1.20
PL-P-4	856	1145	1.34
PL-W-1	611	730	1.19
PL-W-2	681	815	1.20
PL-W-3	720	867	1.20
PL-W-4	801	960	1.20

Table S4. Molecular weight of lignin-like substances.

Samples	M_n (g/mol)	M_w (g/mol)	PDI (M_w/M_n)
LL-M-1	775	1049	1.33
LL-M-2	709	945	1.33
LL-M-3	625	783	1.25
LL-M-4	507	570	1.13
LL-P-1	579	640	1.11
LL-P-2	829	1143	1.34
LL-P-3	777	1049	1.32
LL-P-4	607	753	1.25
LL-W-1	644	811	1.26
LL-W-2	714	964	1.33
LL-W-3	710	944	1.32
LL-W-4	669	832	1.23

Table S5. Correlations between enzymatic hydrolysis yield and various lignin

properties.

	72-hour enzymatic hydrolysis yield	Molecular weight	Contents of phenolic hydroxyl groups	ζ-potential	Contact angles	Relative enzyme activity
Pearson Correlation	1	0.147	-0.911	-0.558	-0.955	0.983
Significance (two-tailed)	-	0.781	0.014	0.251	0.003	0.001

Table S6. Kinetic parameters (V_{max}, K_m) of PL and LL.

| Samples	V_{max}(mg/mL/min)	K_m(mg/mL)	R^2
PL-M-1	0.02537+0.00124	10.57+1.83	0.9811
PL-P-1	0.02230+0.00139	12.83+2.43	0.9750
PL-W-1	0.02098+0.00143	12.95+2.60	0.9591
Avicel	0.01741+0.00188	13.90+2.42	0.9906
LL-M-1	0.01595+0.00156	15.06+2.27	0.9750
LL-P-1	0.01388+0.00267	16.37+2.33	0.9594
LL-W-1	0.01015+0.00089	17.83+2.74	0.9679
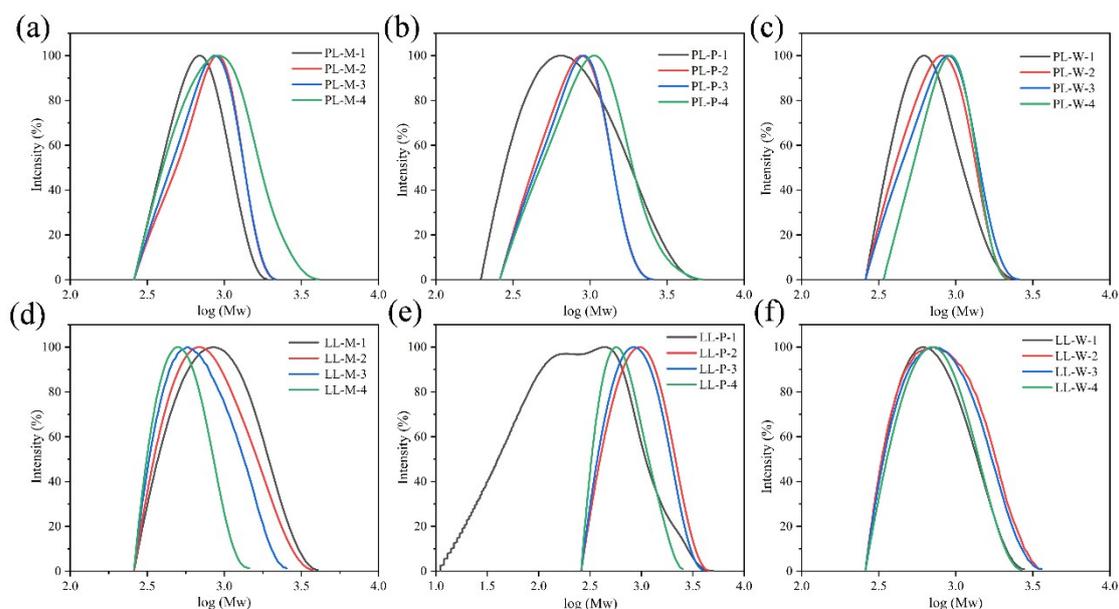
Fig. S1 Molecular weight distribution curves of pseudo-lignin for (a) mason pine, (b) poplar, and (c) wheat straw. Molecular weight distribution curves of lignin-like substances for (d) mason pine, (e) poplar, and (f) wheat straw.
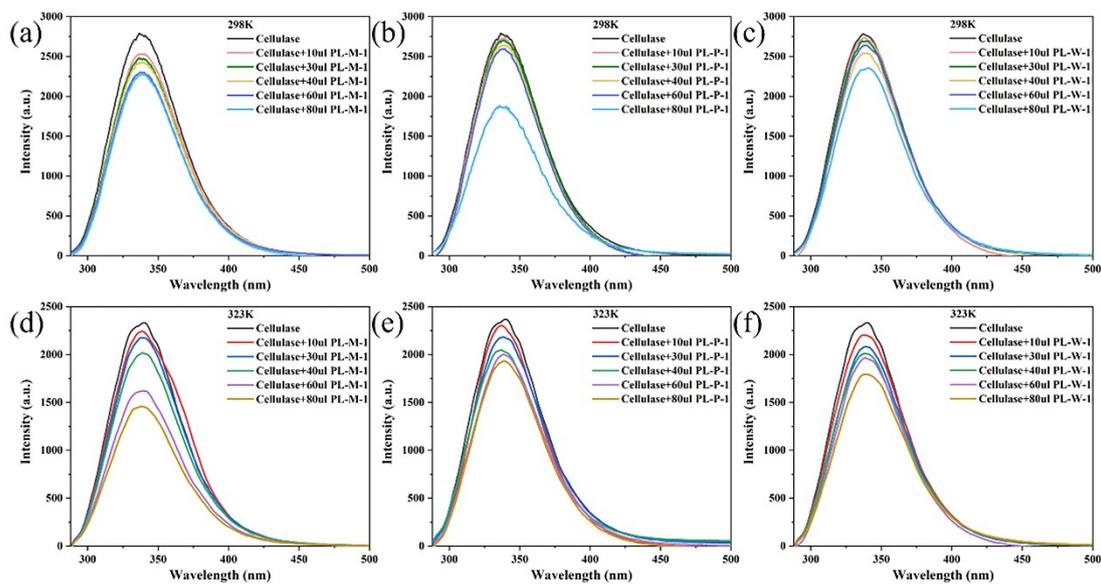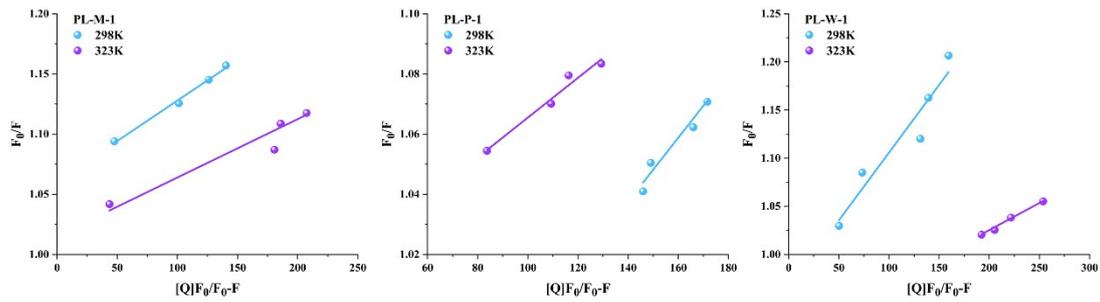

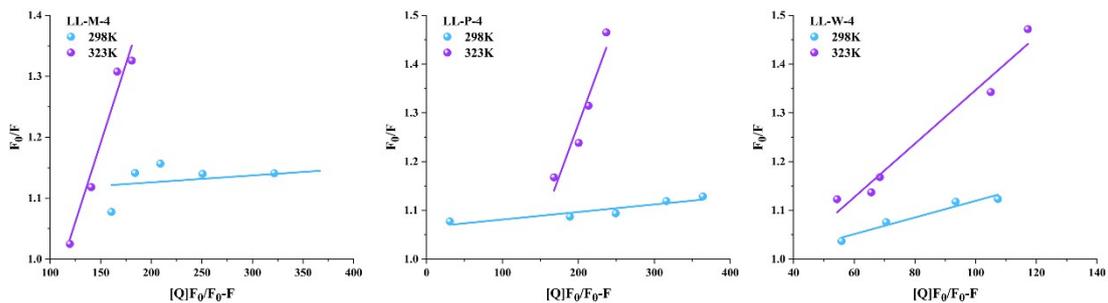**Fig. S2** Effect of pseudo-lignin on fluorescence spectra of cellulase.
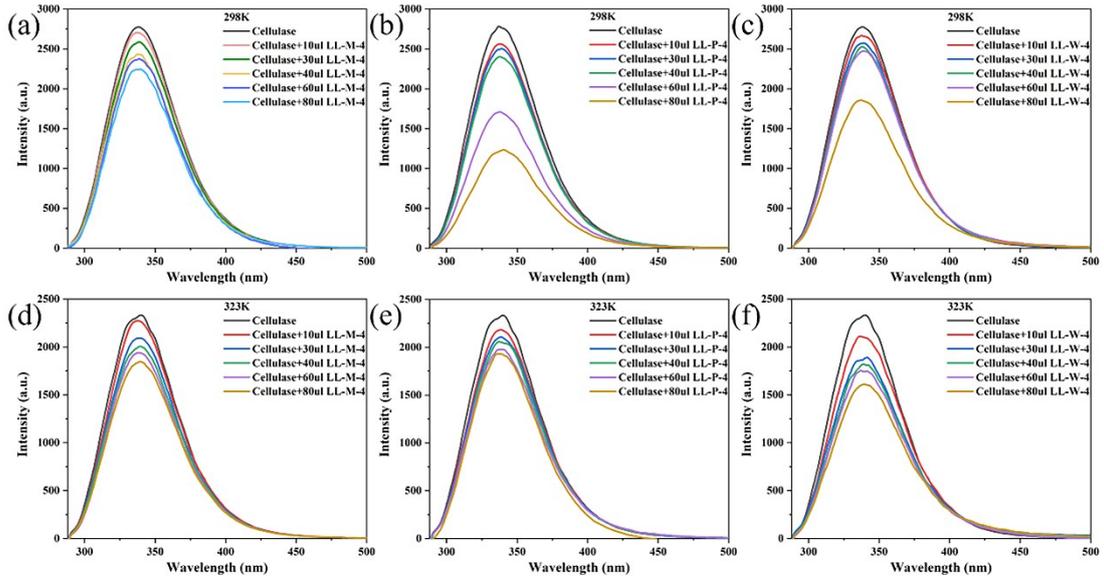
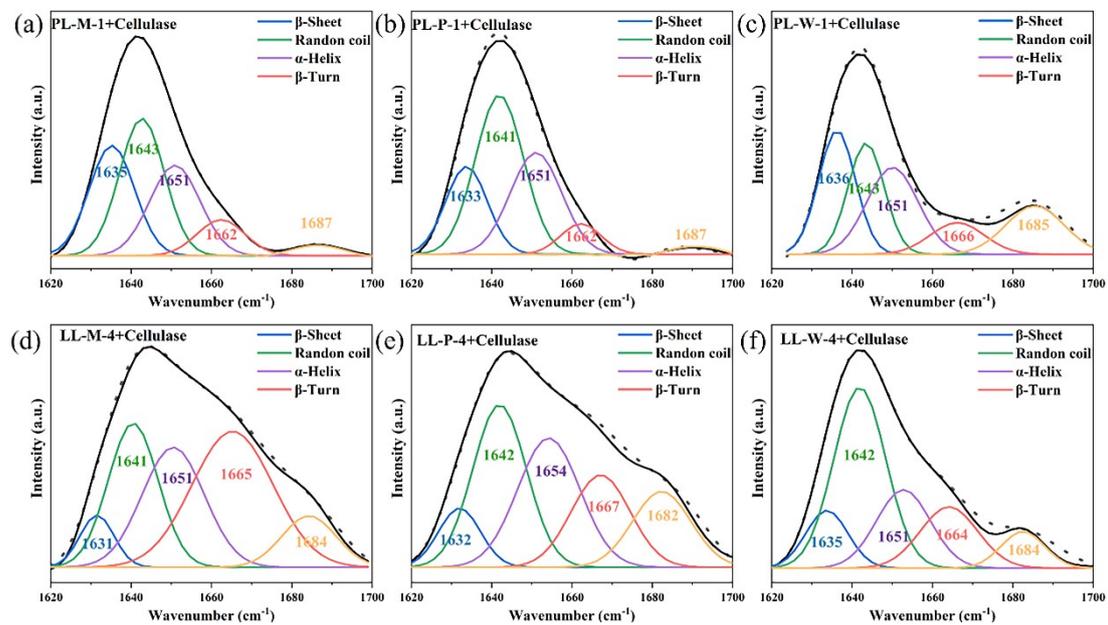**Fig. S3** Effect of lignin-like substances on fluorescence spectra of cellulase.
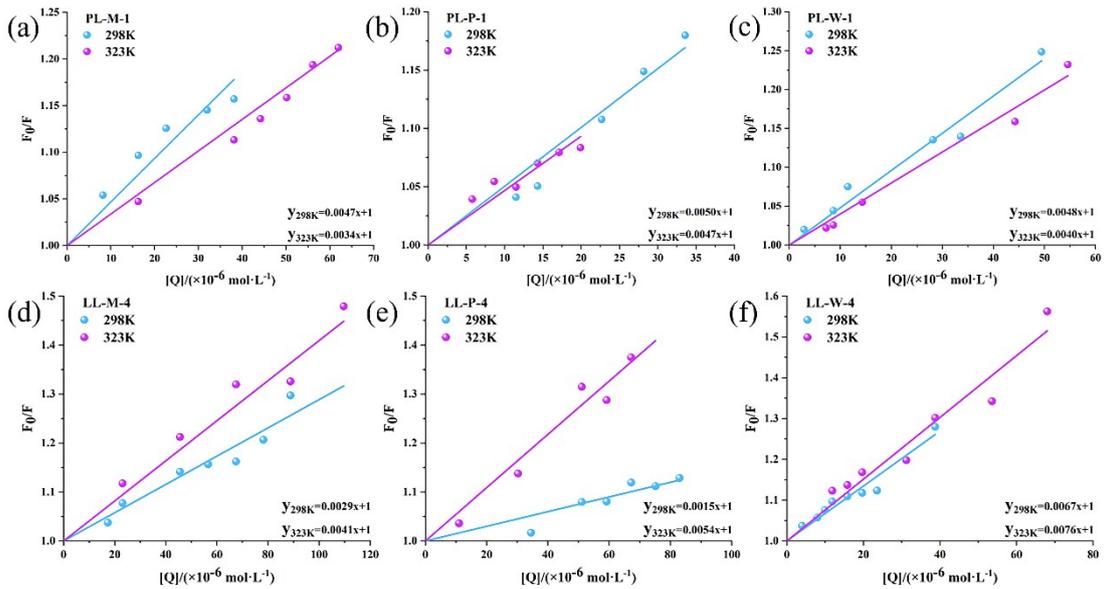
Fig. S4 Stern-Volmer plots of lignin and cellulase system, (a) PL-M, (b) PL-P, (c) PL-W, (d) LL-M, (e) LL-P, (f) LL-W.
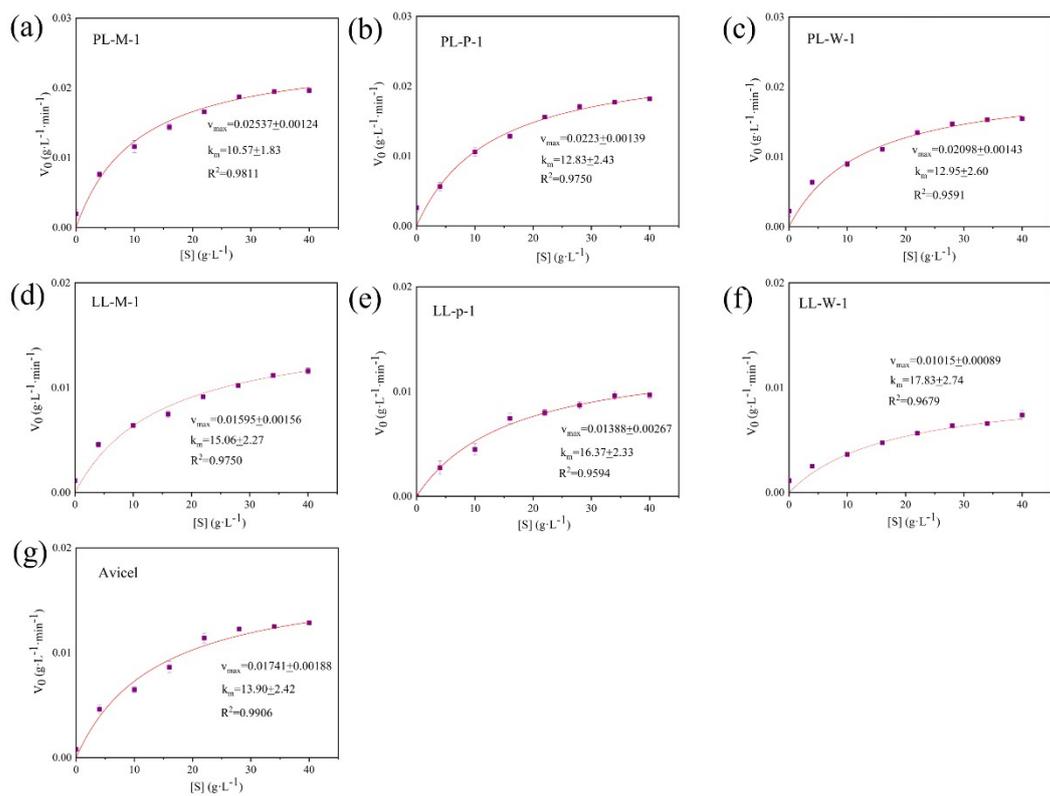
Fig. S5 Scatchard plot of binding constants (Ka) of cellulase to pseudo-lignin.

Fig. S6 Scatchard plot of binding constants (Ka) of cellulase to lignin-like substances.

Fig. S7 Infrared peaks diagram of lignin-cellulase complexes.

Fig. S8 Michaelis–Menten kinetic curves of PL (a-c), LL (d-f), and blank group (g).