Supporting Information

Hydrolytic depolymerization of corncob lignin in the view of the bio-based rigid polyurethane foam synthesis

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Table S1

Assignments of major components in the 2D-HSQC spectra of the original lignin and the DL sample obtained under the optimum condition.

Label	δ_C/δ_H (ppm)	Assignments
$-OCH_3$	55.7/3.70	C−H in methoxyls
A_γ	59.5/3.68	C_γ−H_γ in β-*O*-4 substructures (A)
B_γ	62.3/3.70	C_γ-H_γ for phenylcoumaran (β-5′)(B)
A_α	71.8/4.86	C_α−H_α in β-*O*-4 linked to a S units (A)
A_β(S)	85.8/4.12	C_β−H_β in β-*O*-4 linked to a S units (A)
$S_{2,6}$	103.8/6.70	$C_{2,6}$−$H_{2,6}$ in syringyl units (S)
FA_2	110.8/7.35	C_2-H_2 in ferulates (FA)
G_2	110.8/6.97	C_2−H_2 in guaiacyl units (G)
G_5	114.5/6.70	C_5−H_5 in guaiacyl units (G)
FA_8	116.5/6.36	C_8-H_8 in ferulates (FA)
G_6	119.0/6.78	C_6−H_6 in guaiacyl units (G)
FA_6	122.1/7.20	C_6-H_6 in ferulates (FA)
$H_{2,6}$	127.2/7.12	$C_{2,6}$−$H_{2,6}$ in *p*-hydroxyphenyl units (H)
p-$CA_{2,6}$	130.2/7.48	$C_{2,6}$-$H_{2,6}$ in p-coumarates (*p*-CA)
p-CA_7	144.8/7.51	C_7-H_7 in p-coumarates (*p*-CA)

Table S2

^{31}P NMR spectra analysis of the DL sample obtained under the optimum condition.

Sample	Aliphatic-OH	CS	NCS	CG	NCG	NCH	COOH	total-OH
DL	0.12	0.28	0.40	0.21	1.87	1.62	0.59	5.1

[a]CS, condensed syringyl OH; NCS, noncondensed syringyl OH; CG, condensed guaiacyl OH; NCG noncondensed guaiacyl OH; and NCH, noncondensed p-hydroxyphenyl OH.

Table S3

GC–MS analysis of DCM-soluble fraction obtained under the optimum condition.

Peak number	Retention time (min)	Compound name	Relative content by percent area
1	5.874	n-Propyl acetate	2.15%
2	7.310	Trichloromethane	0.73%
3	27.105	Acetic acid	6.09%
4	27.771	Ethanedioic acid, diethyl ester	0.33%
5	27.946	1-Hexanol, 2-ethyl-	0.21%
6	32.592	Diethyl methylsuccinate	0.63%
7	33.607	Butanedioic acid, diethyl ester	11.67%
8	36.500	Pentanedioic acid, diethyl ester	22.66%
9	39.546	Diethyl adipate	2.02%
10	39.956	Butylated Hydroxytoluene	0.24%
11	42.151	Diethyl pimelate	0.38%
12	42.438	Phenol	1.12%
13	44.264	p-Cresol	0.66%
14	44.464	Diethyl suberate	0.42%
15	46.407	Phenol, 4-ethyl-	0.35%
16	48.028	Hexadecanoic acid, ethyl ester	0.24%
17	50.438	Diethyl Phthalate	0.34%
18	51.135	Ethyl hydrogen succinate	8.14%
19	54.879	Hexanedioic acid, monoethyl ester	0.68%
20	57.628	Catechol	3.55%
Total area (%)			62.61%

[a]The matching degree of all the compounds here were more than 80%, and the compounds whose matching degree less than 80% were not listed.

Figure Captions

Fig. S1. The detailed flow diagram of the separation process for the reaction products.

Fig. S2. FT-IR spectra of the original lignin and DL sample obtained under the optimum condition.

Fig. S3. ^{31}P NMR spectra of DL sample obtained under the optimum condition.

Fig. S4. Degradation TGA curves (a) and the rate of weight loss (b) of original lignin and DL sample obtained under the optimum condition.

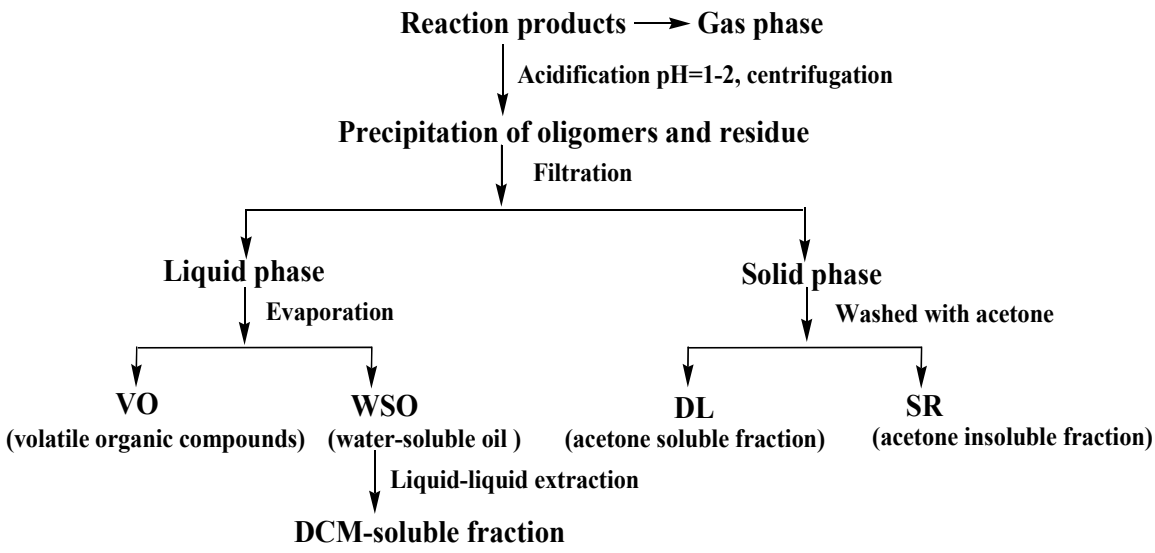
Reaction products
Gas phase
Acidification pH=1-2, centrifugation
Precipitation of oligomers and residue
Filtration
Liquid phase
Solid phase
Evaporation
Washed with acetone
VO
(volatile organic compounds)
WSO
(water-soluble oil)
DL
(acetone soluble fraction)
SR
(acetone insoluble fraction)
Liquid-liquid extraction
DCM-soluble fraction

Fig. S1.

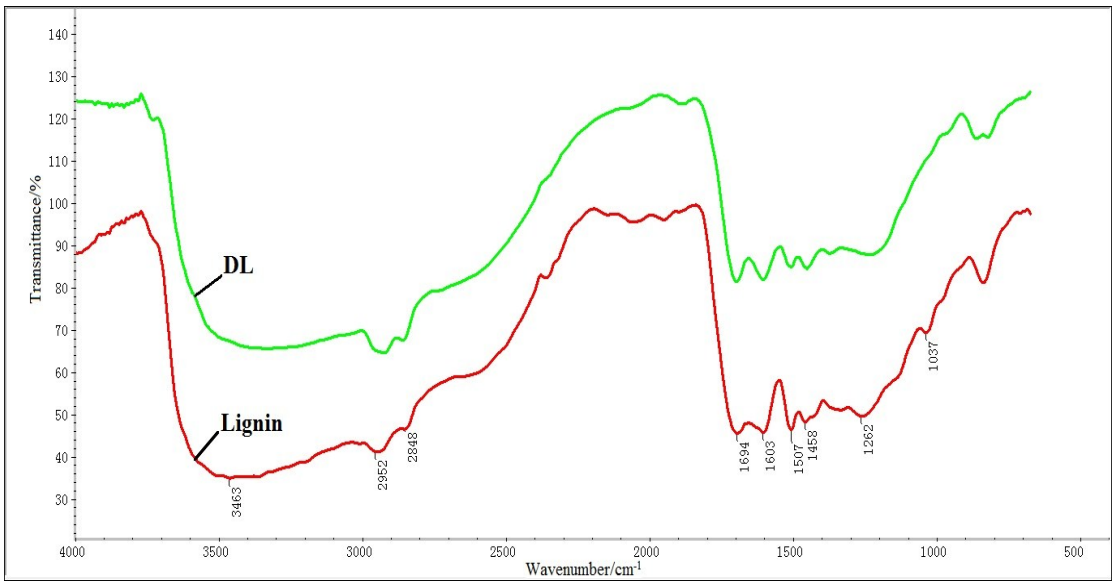
Transmittance/%
Wavenumber/cm-1
DL
Lignin
3463
2952
2848
1694
1603
1507
1458
1262
1037

Fig. S2.

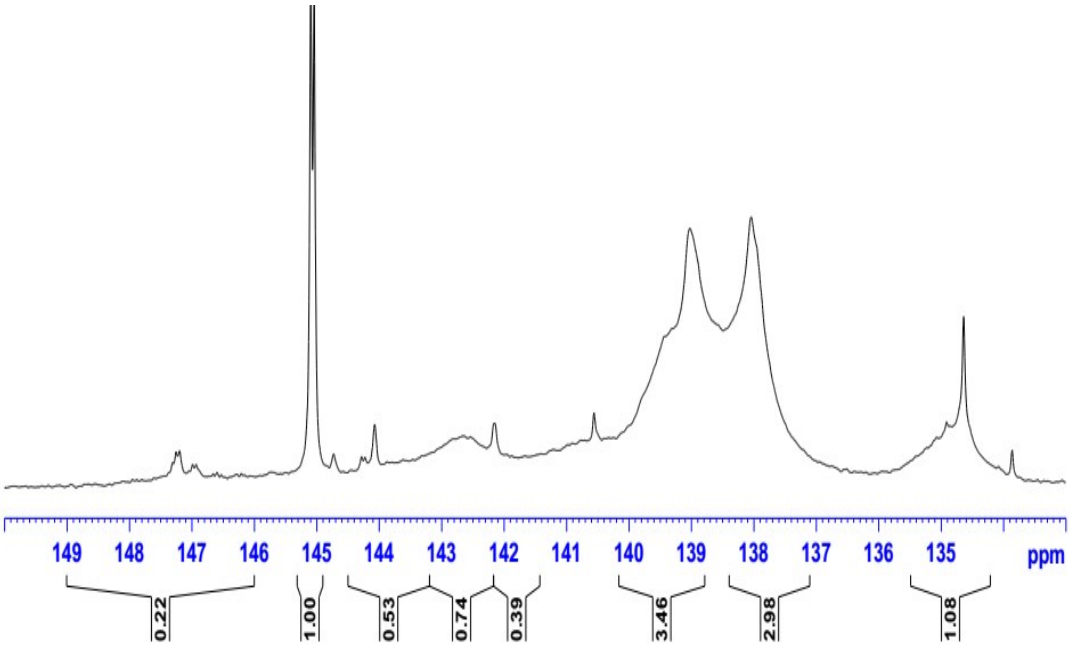
149
148
147
146
145
144
143
142
141
140
139
138
137
136
135
ppm
0.22
1.00
0.53
0.74
0.39
3.46
2.98
1.08

Fig. S3.

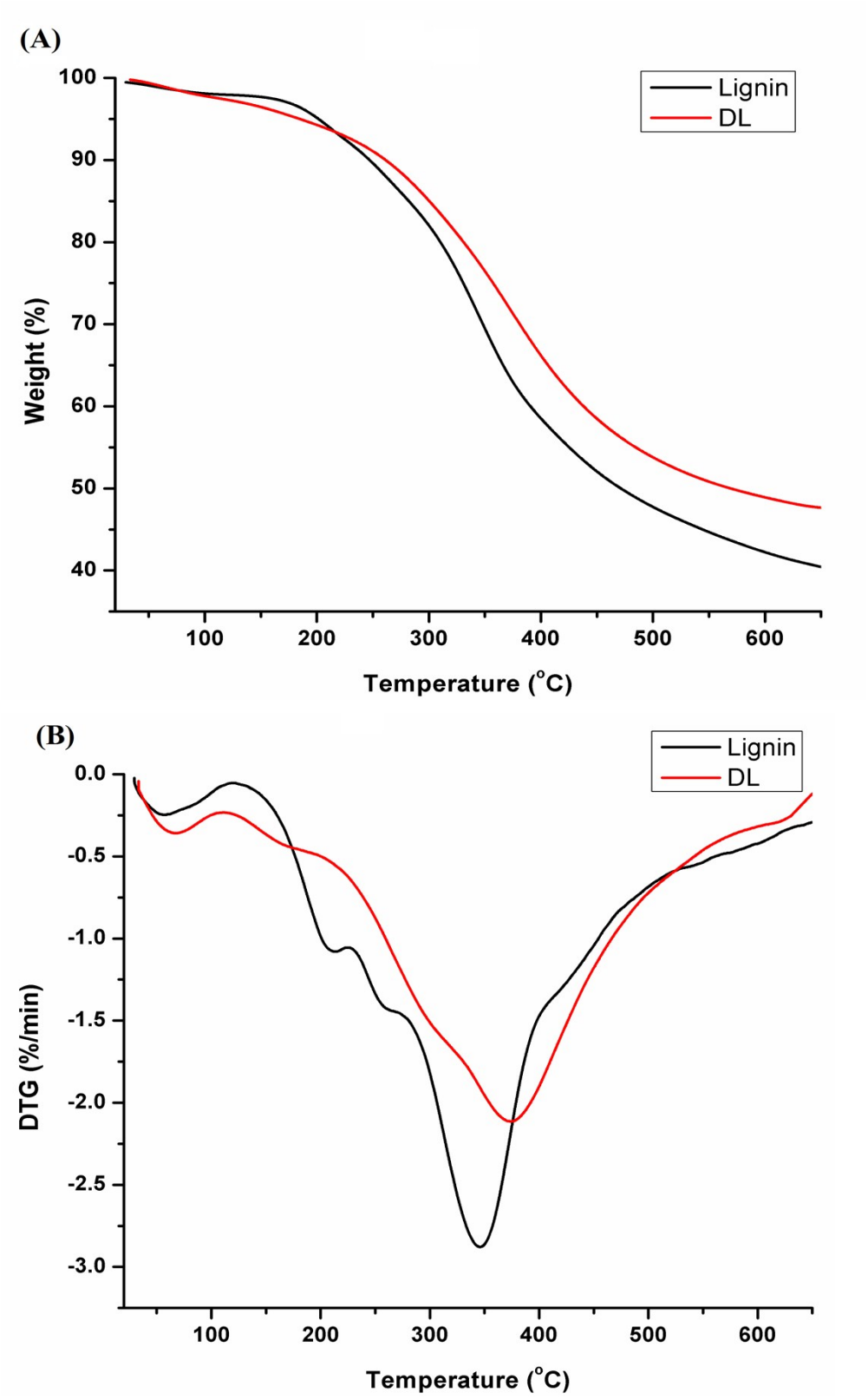
(A)
Lignin
DL
Weight (%)
Temperature (°C)
(B)
Lignin
DL
DTG (%/min)
Temperature (°C)

Fig. S4.