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Supplementary Materials

Effect of Ternary Deep Eutectic Solvents on Bagasse Cellulose and Lignin Structure in Low-Temperature Pretreatment

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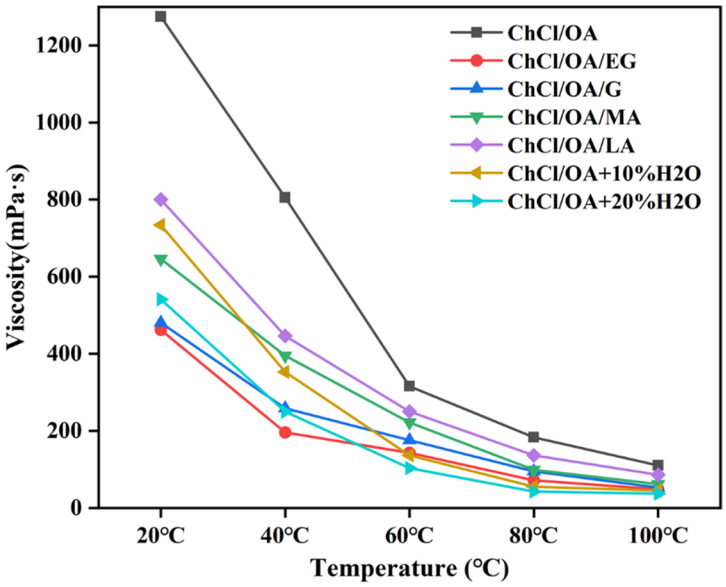

Figure S1. Effect of temperature on the viscosity of different ternary DES.

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Table S1. The viscosity of different ternary DES at 90 °C.

Pretreatment Solvent	ChCl-OA	ChCl-OA-EG	ChCl-OA-G	ChCl-OA-MA	ChCl-OA-LA	ChCl-OA+10% H_2O	ChCl-OA+20% H_2O
Viscosity (mPa·s)	146.3	60.1	72.9	75.3	109.8	50.7	38.2

Table S2. The pH value of different ternary DES.

Pretreatment Solvent	ChCl-OA	ChCl-OA-EG	ChCl-OA-G	ChCl-OA-MA	ChCl-OA-LA	ChCl-OA+10% H2O	ChCl-OA+20% H2O
pH (20 °C)	2.33	3.02	3.22	2.22	2.31	2.39	2.45
pH (60 °C)	1.74	2.40	2.61	1.56	1.72	1.77	1.83

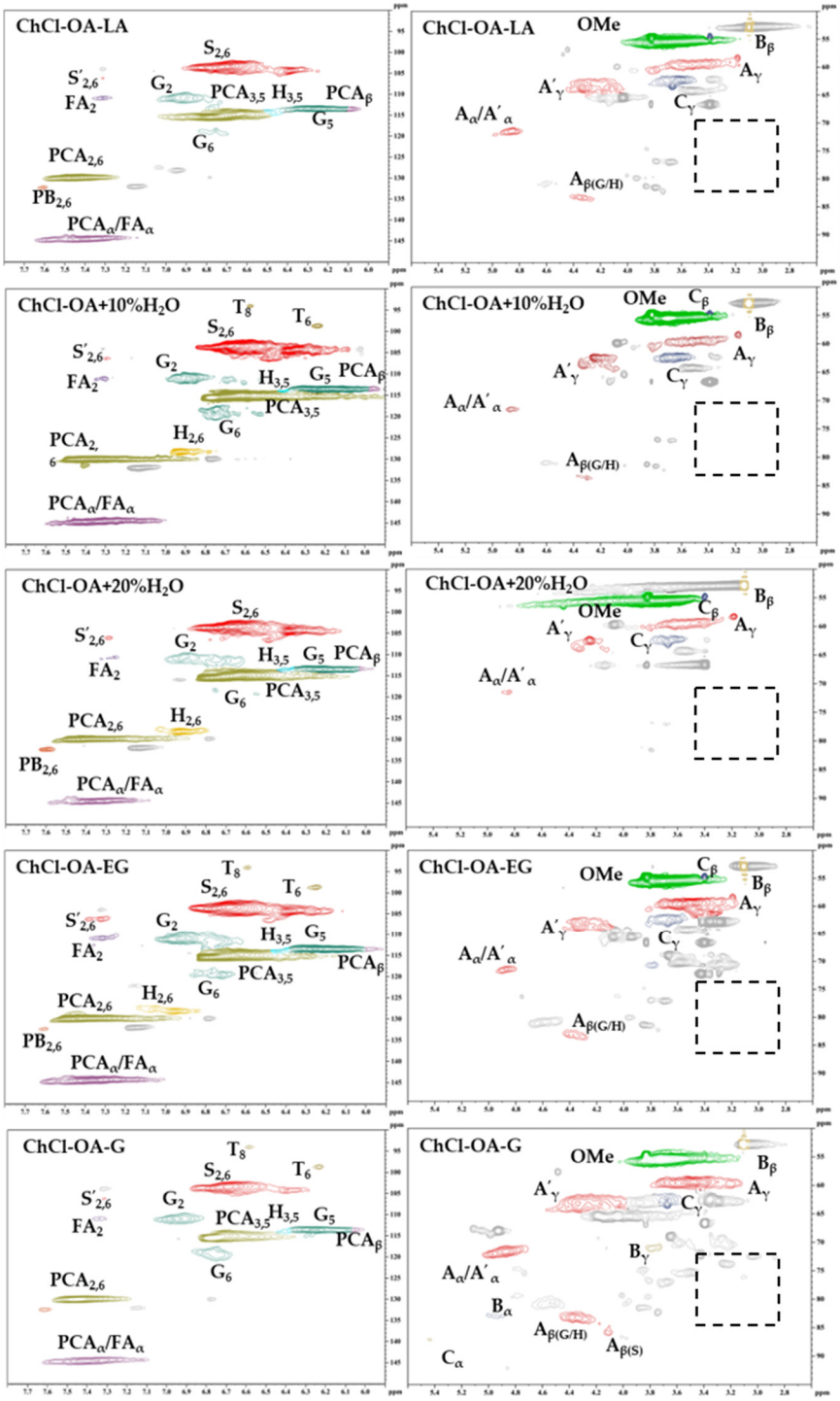

Figure S2. 2D-HSQC NMR spectra of the other DES-L from bagasse.

Table S3. Band assignments for FTIR spectra.

Band (cm^{-1})	Assignment
3385	O-H vibrations
2936	-CH stretching on CH_3 and CH_2
1730	C-O stretch in unconjugated ketone and carboxyl group
1596	Aromatic skeletal vibration breathing with C=C stretching
1512	Aromatic skeletal vibration
1462	-CH asymmetric deformation

1423	Aromatic skeletal vibrations
1325	Syringyl ring breathing with C-O stretching
1270	Aromatic C-O stretching
1209	Guaiacyl ring breathing with C-O stretching
1162	C-O stretch in ester groups
1125	-CH in plane deformation in syringyl ring
1036	-CH in plane deformation in guaiacyl and CO deformation in primary alcohols
831	Aromatic out of plane deformation

Table S4. Assignments of ^{13}C-^{1}H cross-peaks in 2D HSQC spectra of the lignin fractions.

Label	δ_C/δ_H	Assignment
B_β	53.7/3.07	C_β-H_β in β-β′ (resinol) substructures (A)
C_β	53.9/3.45	C_β-H_β in phenylcoumaran substructures (C)
OMe	55.5/3.75	C-H in methoxyl
A_γ	60.2/3.62	C_γ-H_γ in β-O-4′ substructures (A)
B_γ	62.6/3.68	C_γ-H_γ in β-5′ phenylcoumaran substructures (B)
A'_γ	64.6/4.21	C_γ-H_γ in γ-acylated β-O-4′ substructures (A′)
C_γ	71.0/3.70-4.15	C_γ-H_γ in β-β′ resinol substructures (C)
A_α	72.2/4.87	C_α-H_α in β-O-4′ substructures (A)
A'_α	81.4/4.76	C_α-H_α in α-etherified β-O-4 units
$A_{\beta(G)}$	83.1/4.35	C_β-H_β in β-O-4 linked to G/H unit (A)
B_α	83.2/4.9	C_α-H_α in β-β′ phenylcoumaran substructures (B)
$A_{\beta(S)}$	86.6/4.14	C_β-H_β in β-O-4 linked to an S unit (A)
C_α	84.2/5.46	C_α-H_α in phenylcoumaran substructures (C)
T_8	94.7/6.58	C_8–H_8 in tricin (T)
T_6	99.2/6.32	C_6–H_6 in tricin (T)
$S_{2,6}$	104.5/6.72	$C_{2,6}$-$H_{2,6}$ in syringyl units (S)
$S'_{2,6}$	108.7/7.41	$C_{2,6}$-$H_{2,6}$ in oxidized S units (S′)
G_2	116.6/7.01	C_2-H_2 in guaiacyl units (G)
G_5	115.2/6.72	C_5-H_5 in guaiacyl units (G)
G_6	119.7/6.81	C_6-H_6 in guaiacyl units (G)
$H_{3,5}$	114.5/6.62	$C_{3,5}$-$H_{3,5}$ in *p*-hydroxyphenyl units (H) and Proteins
PCA_β/FA_β	114.5/6.48	C_β–H_β in *p*-coumarates (PCA) and ferulates (FA)
$PCA_{3,5}$	116.3/6.80	$C_{3,5}$-$H_{3,5}$ in *p*-coumaric acid (PCA)
FA_2	111.3/7.31	C_2–H_2 in ferulate (FA)
$H_{2,6}$	127.7/7.21	$C_{2,6}$–$H_{2,6}$ in *p*-hydroxyphenyl units (H) and proteins
$PCA_{2,6}$	130.72/7.47	$C_{2,6}$–$H_{2,6}$ in *p*-coumarates (PCA)
PCA_α/FA_α	145.3/7.43	C_α–H_α in *p*-coumarates (PCA) and ferulates (FA)
$PB_{2,6}$	133.1/7.63	$C_{2,6}$–$H_{2,6}$ in *p*-Hydroxybenzoate
FA_2	111.3/7.31	C_2–H_2 in ferulate (FA)

Table S5. The TG analysis of bagasse treated with different DESs.

Pretreatment Solvent	Mass loss (%)		T_{onset}/ °C	T_{max}/ °C
	50-310°C	310-500°C		
Raw	23.37	78.49	213.2	339.3
ChCl-OA-EG	16.73	90.07	218.5	358.9
ChCl-OA-G	16.21	89.13	217.9	359.1
ChCl-OA-LA	14.70	89.03	220.3	355.1
ChCl-OA-MA	13.14	92.73	222.6	357.6

ChCl-OA+10% H_2O	17.77	86.90	218.3	354.9
ChCl-OA+20% H_2O	13.27	86.30	219.7	356.8

T_{onset}/°C, the pronounced decomposition onset temperature. T_{max}/°C, the maximum decomposition rate temperature.

Table S6. The TG analysis of different DES-Ls.

Pretreatment Solvent	Mass loss (%)		T_{onset}/ °C	T_{max}/ °C
	50-300°C	300-600°C		
Raw	32.64	79.86	201.1	290.6
ChCl-OA-EG	34.72	69.82	206.3	261.2
ChCl-OA-G	33.16	70.41	200.8	237.3
ChCl-OA-LA	19.94	59.13	214.1	358.1
ChCl-OA-MA	21.14	62.01	190.4	357.2
ChCl-OA+10% H_2O	26.32	57.65	200.6	265.1
ChCl-OA+20% H_2O	34.11	68.39	198.4	261.9

T_{onset}/°C, the pronounced decomposition onset temperature. T_{max}/°C, the maximum decomposition rate temperature.