Supporting information

Mild organosolv pretreatment of sugarcane bagasse with acetone/phenoxyethanol/water for enhanced sugar production

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List of supporting information

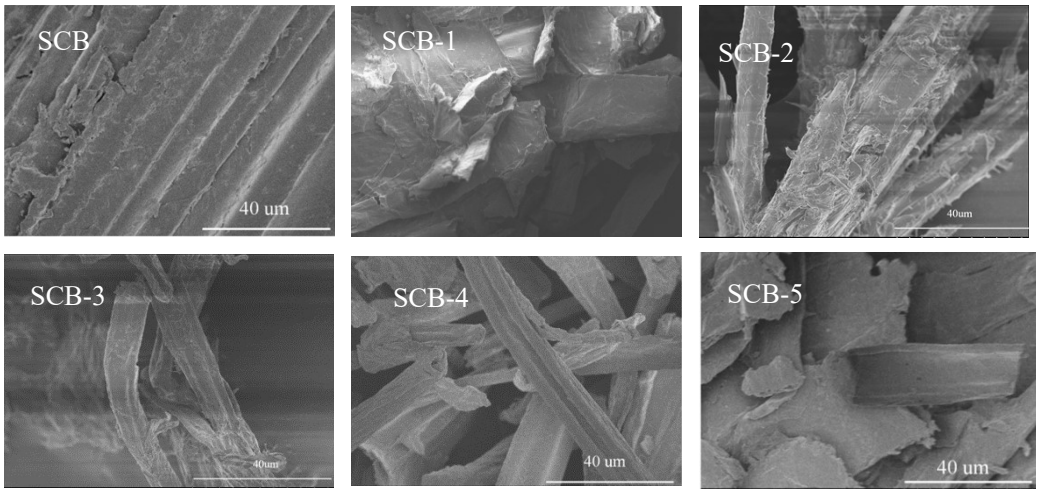

Figure S1 SEM images of raw biomass (SCB) and residues

(SCB-1, 125 ℃ - 120 min - 0.17 M H2SO4 - LSR15;

SCB-2, 110 ℃ - 120 min - 0.15 M H2SO4 - LSR10;

SCB-3, 110 ℃ - 110 min - 0.1 M H2SO4 - LSR10;

SCB-4, 110 ℃ - 80 min - 0.2 M H2SO4 - LSR10;

SCB-5, 110 ℃ - 90 min - 0.15 M H2SO4 - LSR10).

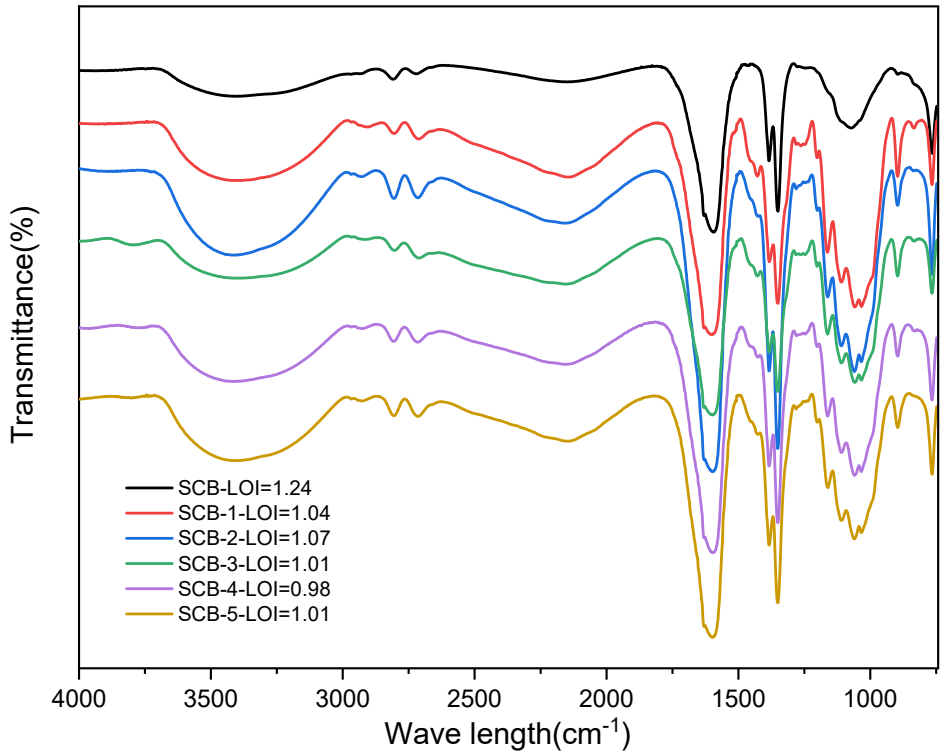

Figure S2 FTIR of raw biomass and residues (LOI=A1430cm-1/A898cm-1)

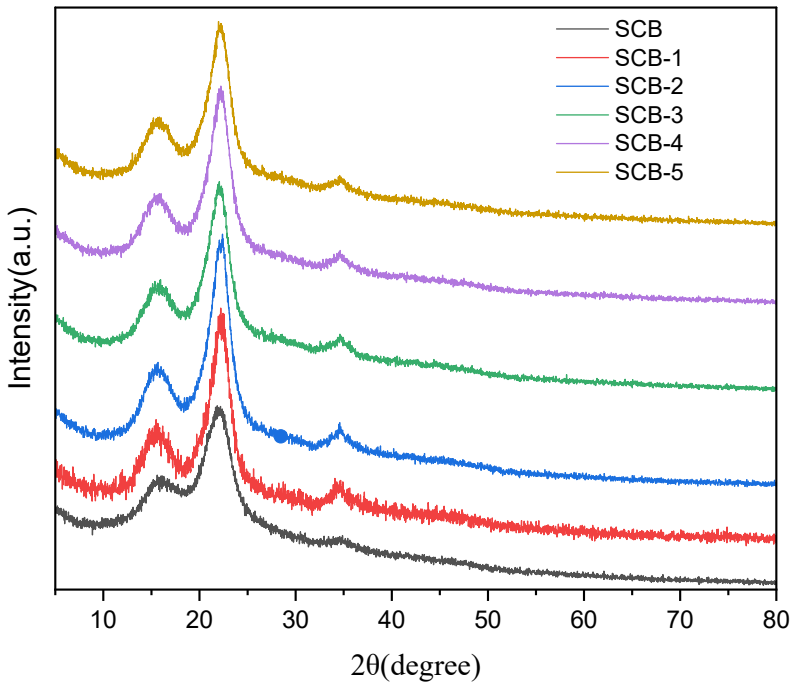

Figure S3 XRD of raw biomass and residues

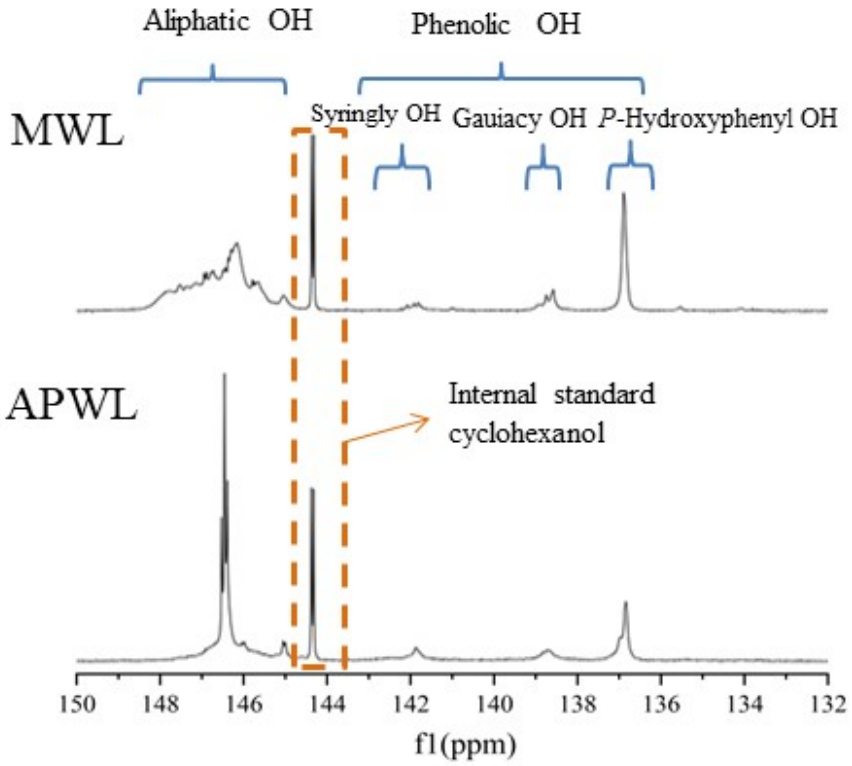

Figure S4 Quantitative ^{31}P NMR spectrum of MWL and APWL derivatized with TMDP using cyclohexanol as internal standard

Table S1 Four-fraction Box-Behnken design

Symbol	Variable	Coding level		
		-1	0	1
X_1	Time, min	30	75	120
X_2	Temperature,℃	80	105	130
X_3	H_2SO_4, M	0.05	0.175	0.3
X_4	L:S	10	15	20

Table S2 Variance analysis of the quadratic model

Source	Sum of squares	df	Mean square	F value	p-value Prob>F	Remarks
Model	18158.1	14	1297	22.52	0.000	significant
X_1	1657.5	1	1657.5	28.78	0.000	significant
X_2	11660.1	1	11660.1	202.46	0.000	significant
X_3	2167.9	1	2167.9	37.64	0.000	significant
X_4	5.7	1	5.7	0.1	0.758	
X_1^2	90.6	1	90.6	1.57	0.230	
X_2^2	1955.3	1	1955.3	33.95	0.000	significant
X_3^2	440.0	1	440.0	7.64	0.015	
X_4^2	105.7	1	105.7	1.84	0.197	
$X_1 X_2$	49.8	1	49.8	0.87	0.368	
$X_1 X_3$	281.4	1	281.4	4.89	0.044	
$X_1 X_4$	14.9	1	14.9	0.26	0.619	
$X_2 X_3$	164.0	1	164.0	2.85	0.114	
$X_2 X_4$	22.3	1	22.3	0.39	0.544	
$X_3 X_4$	13.7	1	13.7	0.24	0.634	
Residual	806.3	14	57.6			
Lack of fit	792.3	10	79.2	22.65	0.004	
Pure error	14.0	4	3.5			
Cor Total	18964.4	28				

Table S3 Comparison of treatment with APW to that with other organsolv solvents

Plant species	Pretreatment conditions	Lignin removal rate	Reference
Sugarcane bagasse	APW, 0.2 M H2SO4, 110 ℃, 80min,	94.94%	This study
Sugarcane bagasse	50% ethanol + BHT, 20% H2SO4, 120℃, 30min	72.45%	[1]
Sugarcane bagasse	Water/1-buthanol (4.0mol/mol), 200℃,	67%	[2]
Rice straw	70% EPH:30%H2O, 0.05M H2SO4, 130℃, 2h	63.16%	[3]
Corncob	60 % pentanol, 160 ℃, 60 min	85%	[4]

Reference

[1] A. A. Schmatz and M. Brienzo, BioEnergy Research, 2021, 15, 166-174.

[2] Y. Kawamata, T. Yoshikawa, Y. Koyama, H. Ishimaru, S. Ohtsuki, E. Fumoto, S. Sato, Y. Nakasaka and T. Masuda, Industrial Crops and Products, 2021, 159.113078.

[3] Q. Zhang, Y. Deng, X. Tan, W. Wang, Q. Yu, X. Chen, C. Miao, Y. Guo, Y. Zhang, X. Zhuang and Z. Yuan, Industrial Crops and Products, 2020, 145.112091.

[4] M. Madadi, Zahoor, G. J. Song, K. Karimi, D. C. Zhu, M. Elsayed, F. B. Sun and A. Abomohra, Bioresource Technology, 2022, 359.127503.

Table S4 The assignment of peaks in 2D HSQC spectra of MWL and APWL

Label	δ_C/δ_H(ppm)		Assignment
	MWL	APWL	
B'_β	50.49/2.62	ND	C_β–H_β in β-β tetrahydrofuran (B')
B_β	53.36/3.71	54.25/3.69	Cβ–Hβ in β-β tetrahydrofuran (B')
OCH_3	55.44/3.74	56.22/3.67	C-H in methoxyl
A_γ	60.14/3.57	ND	C_γ-H_γ in β-O-4 substructures (A)
B_γ	66.16/3.76	71.77/4.20	C_γ–H_γ in phenylcoumaran substructures (B)
A'_γ	63.95/4.27	ND	C_γ–H_γ in γ-acylated β–O–4 (A')
B_γ	71.77/4.19	69.75/3.97	C_γ–H_γ in β-β resinol (B)
Glc_5	71.47/3.51	ND	C_5-H_5 in cellulose
A_α	72.35/4.85	ND	C_α-H_α in β-O-4 substructures (A)
X_2	72.71/3.21	ND	C_2-H_2 in β-D-xylopyranoside (X)
B'_α	83.57/4.97	ND	C_α–H_α in β-β (B', tetrahydrofuran)
B_α	85.08/4.69	82.13/4.88	C_α–H_α in β-β resinol (B)
X_3	74.94/3.25	ND	C_3-H_3 in β-D-xylopyranoside (X)
X_4	76.14/3.53	ND	C_4-H_4 in xylan substructures (X)
A_β (G)	83.27/4.41	ND	C_β-H_β in β-O-4 substructures linked to G（A）
A_β(S)	86.38/4.13	ND	C_β-H_β in β-O-4 substructures linked to a S unit (A)
T_6	94.75/6.60	ND	$C'_{2,6}$–$H'_{2,6}$ in tricin (T)
T_8	99.38/6.25	ND	$C_{2,6}$–$H_{2,6}$ in tricin (T)
T_3	105.45/7.05	ND	C_8–H_8 in tricin (T)
$S_{2,6}$	104.53/6.72	105.96/6.62	$C_{2,6}$-$H_{2,6}$ in syringyl units (S)
$S'_{2,6}$	107.13/7.34	106.76/7.32	$C_{2,6}$–$H_{2,6}$ in oxidized S units (S')
$T'_{2,6}$	106.49/7.30	ND	$C'_{2,6}$–$H'_{2,6}$ in tricin (T)
G_2	111.64/7.0	ND	C_2-H_2 in guaiacyl units (G)
FA_2	112.02/7.35	111.89/7.32	C_2–H_2 in ferulic acid (FA)
pCE_8	114.20/6.24	114.59/6.29	C_8-H_8 in p-coumarate unites (pCA)
G_5	115.47/6.8	114.28/6.76	C_5-H_5 in guaiacyl units (G)
G_6	119.72/6.84	120.84/6.81	C_6-H_6 in guaiacyl units (G)
$H_{2,6}$	128.51/7.18	129.65/7.16	$C_{2,6}$-$H_{2,6}$ in p-hydroxyphenyl units (H)
$pCE_{2,6}$	130.48/7.46	130.06/7.45	$C_{2,6}$-$H_{2,6}$ in p-coumaric acid (pCA)
pCE_7/FA_7	145.31/7.41	145.08/7.44	C_7-H_7 in p-coumarate unites (pCA) / ferulate units (FA)

Table S5 Hydroxyl group contents of MWL and APWL as determined by ^{31}P NMR analysis

Lignin sample	Aliphatic OH mmol/g	Phenolic OH, mmol/g			COOH mmol/g
		Syringyl	Guaiacyl	p-hydroxy phenyl	
MWL	8.60	0.18	0.53	1.70	ND
APWL	6.12	0.52	0.66	1.86	ND