designs

Supplementary Materials

The Relationship between Structural Features of Lignocellulosic Materials and Ethanol Production yield

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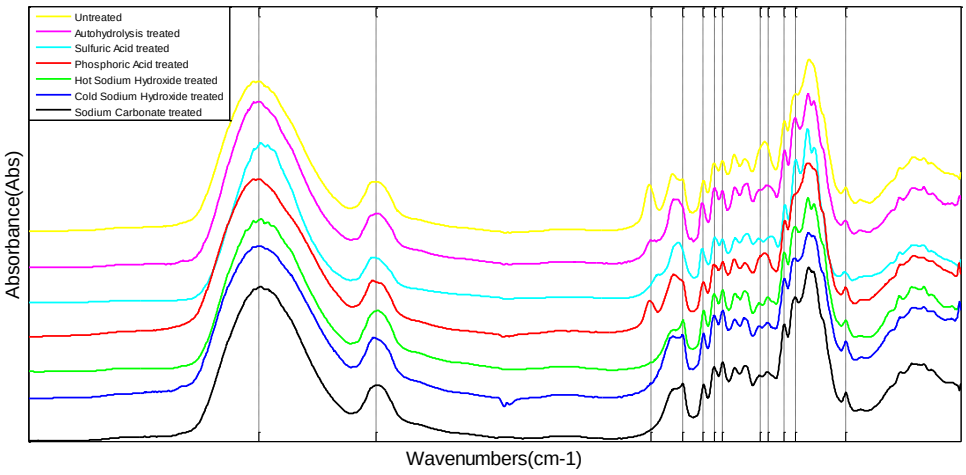

Figure S1: FTIR spectra obtained from scanning untreated and pretreated poplar wood

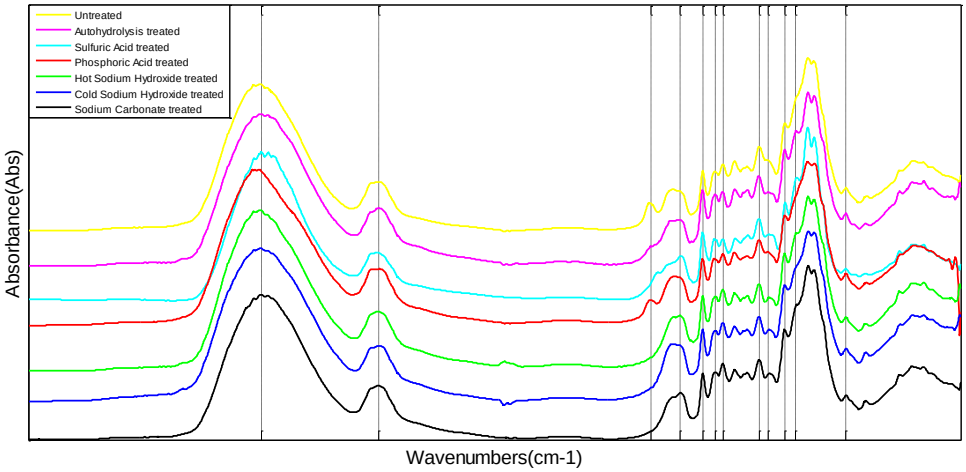

Figure S2: FTIR spectra obtained from scanning untreated and pretreated pinewood

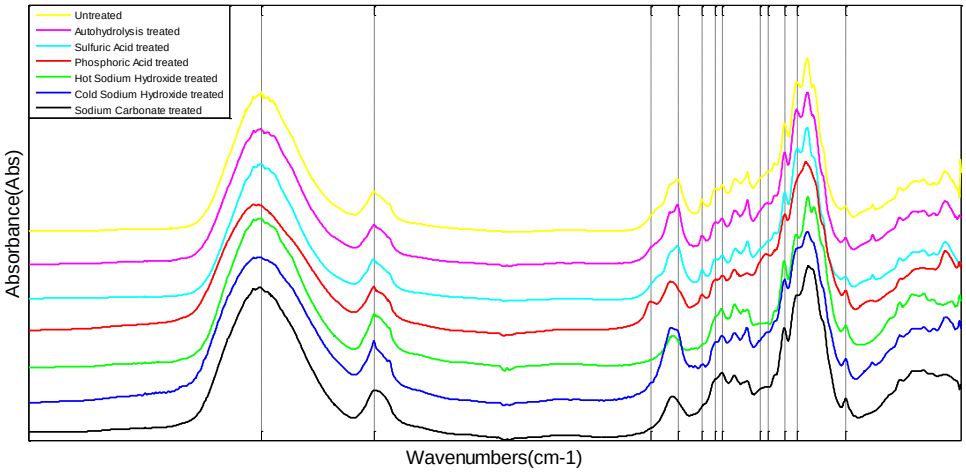

Figure S3: FTIR spectra obtained from scanning untreated and pretreated rice straw

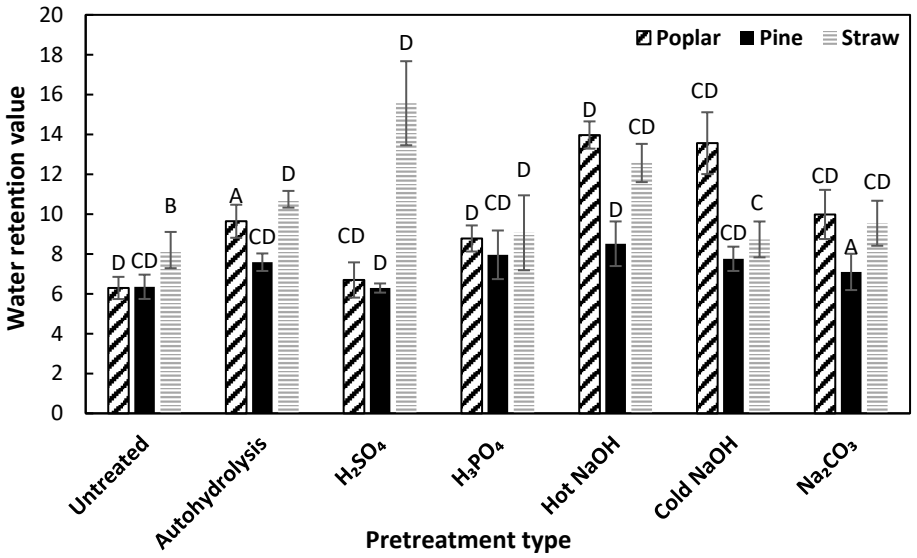

Figure S4: Water retention value of untreated and pretreated substrates using nonwoven bags

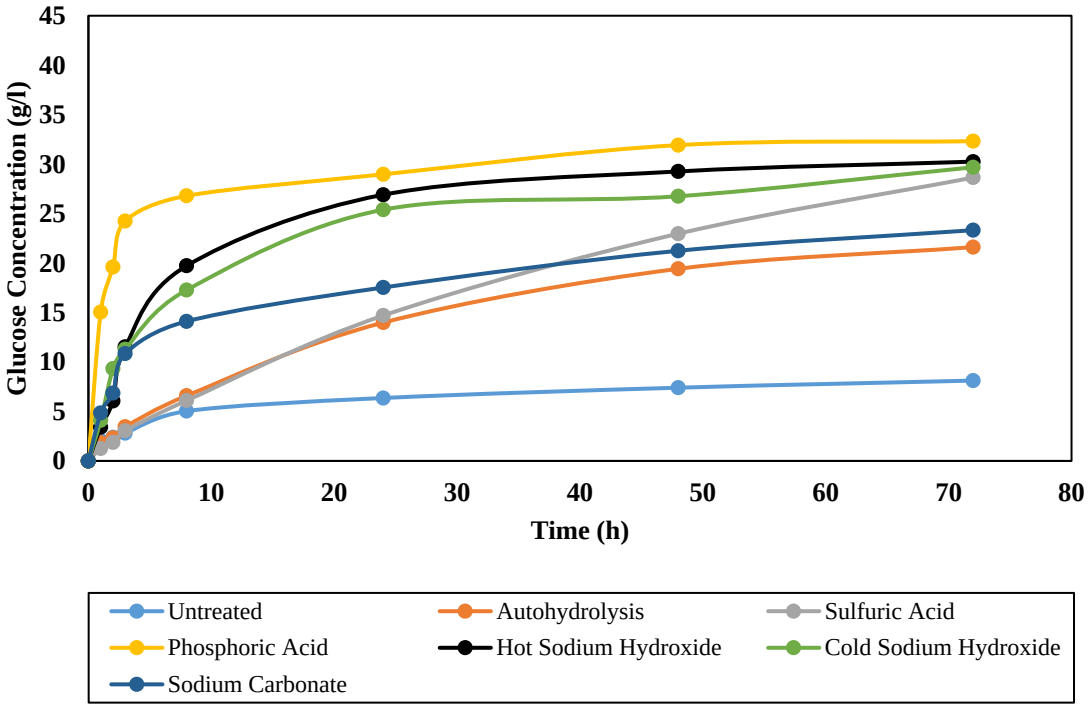

Figure S5: Glucose concentration during enzymatic hydrolysis of untreated and pretreated poplar wood

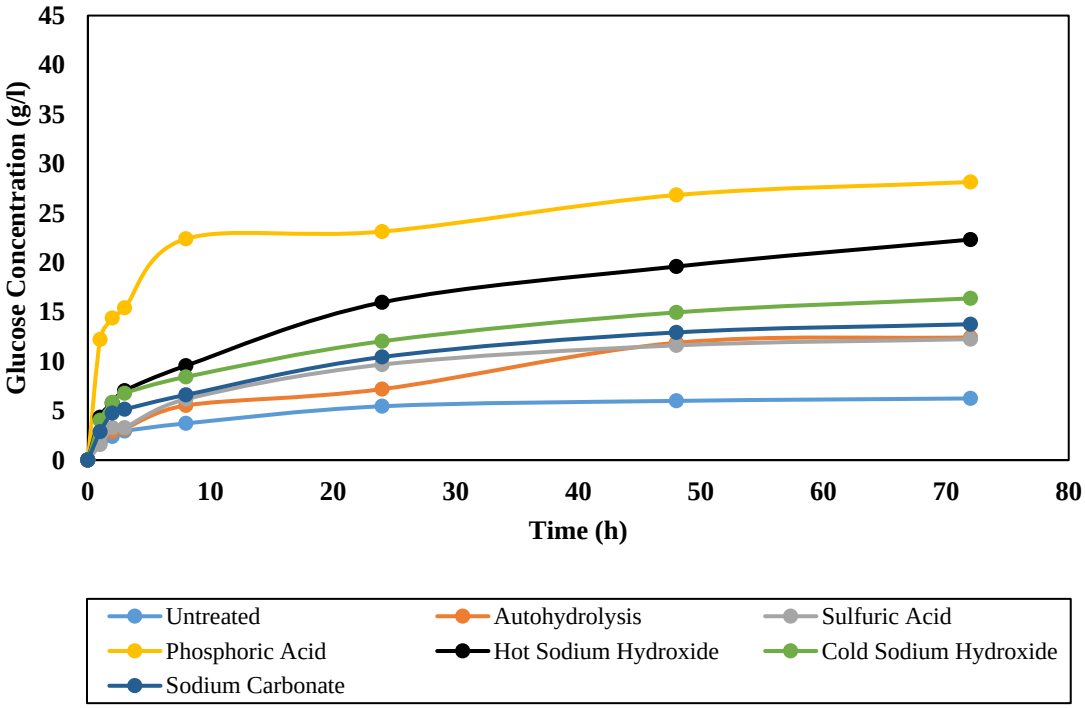

Figure S6: Glucose concentration during enzymatic hydrolysis of untreated and pretreated pinewood

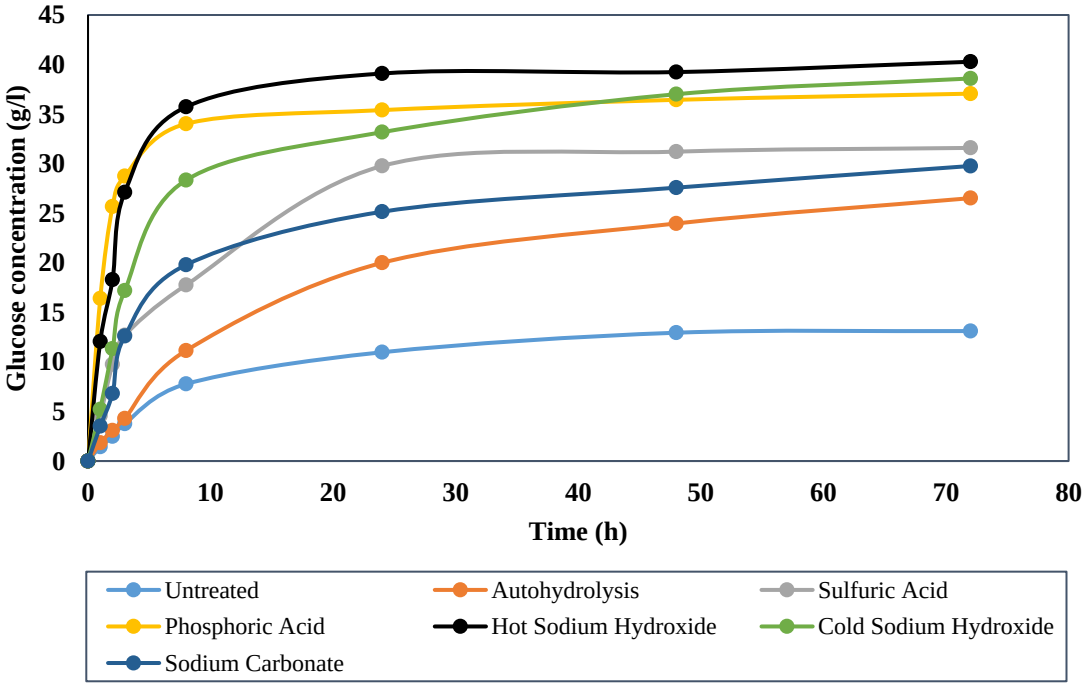

Figure S7: Glucose concentration during enzymatic hydrolysis of untreated and pretreated rice straw

Table S1: Total solids, volatile solids, and pretreatment recovery percentages of substrates

Substrate	Pretreatment Type	Total Solids (%)	Volatile Solids (%)	Recovery (%)
Poplar	Untreated	96.6±0.1	96.3±0.4	-
	Autohydrolysis	96.8±0.3	95.3±0.4	67.8
	Sulfuric Acid	99.6±0.1	98.5±0.3	62.2
	Phosphoric Acid	98.4±0.5	97.7±0.7	76.3
	Hot Sodium Hydroxide	97.1±0.6	97.7±0.5	56.5
	Cold Sodium Hydroxide	96.6±0.5	96.8±0.4	77.4
	Sodium Carbonate	96.7±0.2	95.9±0.6	76.0
Pine	Untreated	97.5±0.2	97.2±0.6	-
	Autohydrolysis	97.2±0.00	98.3±0.1	71.4
	Sulfuric Acid	98.7±0.3	99.0±0.7	61.8
	Phosphoric Acid	98.8±1.0	96.7±0.1	79.3
	Hot Sodium Hydroxide	97.2±0.2	96.5±0.2	76.2
	Cold Sodium Hydroxide	97.6±0.0	96.8±0.1	93.6
	Sodium Carbonate	95.9±0.2	94.5±0.1	84.8
Rice Straw	Untreated	95.8±0.2	88.6±0.3	-
	Autohydrolysis	97.3±0.0	91.2±0.1	57.5
	Sulfuric Acid	97.8±0.5	81.8±0.3	51.1
	Phosphoric Acid	98.2±0.2	85.8±0.5	66.6
	Hot Sodium Hydroxide	97.9±0.2	91.0±0.3	33.2
	Cold Sodium Hydroxide	96.8±0.6	85.9±0.8	66.6
	Sodium Carbonate	96.5±0.1	87.7±0.1	59.3

Table S2: Relative change in adsorption at different wavenumbers after pretreating poplar wood

Band position	Assignment	Pretreatment					
		Au*	H_2SO_4	H_3PO_4	Hot NaOH	Cold NaOH	Na_2CO_3
896	Asym., out of phase ring stretching Cellulose II (895) Amorphous Cellulose (895) Xylan (899)	0.03	-0.34	0.09	0.13	0.43	0.06
1111	Ring asymmetric stretching Cellulose I (1111)	0.07	0.02	-	0.04	0.07	0.04
1160	C-O-C asymmetric stretching Cellulose I (1155) Cellulose II (1162)	0.04	-0.12	0.04	0.07	0.14	0.05
1230	C–O stretching Lignin and hemicellulose (1235)	-0.10	-0.28	-0.08	-0.18	-0.08	-0.24
1265	Guaiacyl rings vibrating (1270)	-0.15	-0.30	-	-0.25	-0.12	-0.28
1425	C–H_2 symmetric bending Cellulose I (1431)	0.06	-0.13	0.03	0.13	0.32	0.09
1459	–OH in plane bending Cellulose I (1455) Cellulose II (1470) Asymmetric bending in C–H_3 Lignin (1465)	0.14	-0.07	0.04	0.11	0.30	0.06
1507	C–C stretching of the aromatic ring Lignin (1510)	0.24	0.03	0.04	0.17	0.40	0.08
1595	C=C Lignin (1595)	0.27	0.12	-	-0.04	0.33	0.07
1732	C=O stretching of acetyl/carboxylic acid/esters/carbonyl Hemicellulose and lignin (1720-1745)	-0.43	-	-0.24	-	-0.52	-
2910	C-H stretching Cellulose I (2900) Cellulose II (2900)	0.06	-0.13	0.10	0.19	0.35	0.10
3413	–OH stretching intramolecular hydrogen bonds Cellulose I (3352) Cellulose II (3447)	0.09	0.05	0.04	0.01	0.06	0.02

*Au: Autohydrolysis

Table S3: Relative change in adsorption at different wavenumbers after pretreating pine wood

Band position	Assignment	Pretreatment					
		Au*	H_2SO_4	H_3PO_4	Hot NaOH	Cold NaOH	Na_2CO_3
896	Asym., out of phase ring stretching Cellulose II (895) Amorphous Cellulose (895) Xylan (899)	0.21	-0.26	0.42	0.23	0.30	0.02
1159	C-O-C asymmetric stretching Cellulose I (1155) Cellulose II (1162)	0.07	-0.09	0.11	0.08	0.11	0.02
1230	C–O stretching Lignin and hemicellulose (1235)	0.04	-0.07	0.17	0.02	0.06	-0.07
1267	Guaiacyl rings vibrating (1270)	0.06	-0.04	0.12	0.01	0.04	-0.05
1423	C–H_2 symmetric bending Cellulose I (1431)	0.11	-0.08	0.21	0.20	0.23	0.14
1455	–OH in plane bending Cellulose I (1455) Cellulose II (1470) Asymmetric bending in C–H_3 Lignin (1465)	0.20	0.03	0.28	0.24	0.25	0.13
1510	C–C stretching of the aromatic ring Lignin (1510)	0.27	0.14	0.28	0.23	0.25	0.10
1606	C=C Lignin (1595)	0.15	0.11	-	0.35	-	0.16
1732	C=O stretching of acetyl/carboxylic acid/esters/carbonyl Hemicellulose and lignin (1720-1745)	-0.31	-	-	-	-	-
2900	C-H stretching Cellulose I (2900) Cellulose II (2900)	0.17	-0.02	0.35	0.19	0.20	0.09
3400	–OH stretching intramolecular hydrogen bonds Cellulose I (3352) Cellulose II (3447)	0.03	0.01	0.08	0.09	0.06	-0.01

*Au: Autohydrolysis

Table S4: Relative change in adsorption at different wavenumbers after pretreating rice straw

Band position	Assignment	Pretreatment					
		Au*	H_2SO_4	H_3PO_4	Hot NaOH	Cold NaOH	Na_2CO_3
898	Asym., out of phase ring stretching Cellulose II (895) Amorphous Cellulose (895) Xylan (899)	0.12	-0.02	0.78	0.78	0.83	0.65
1106	Ring asymmetric stretching Cellulose I (1111)	0.05	0.02	-	-0.09	-	-0.03
1159	C-O-C asymmetric stretching Cellulose I (1155) Cellulose II (1162)	0.05	0.00	0.12	0.01	0.16	0.03
1427	C–H_2 symmetric bending Cellulose I (1431)	0.03	-0.01	0.29	0.32	0.50	0.45
1454	–OH in plane bending Cellulose I (1455) Cellulose II (1470) Asymmetric bending in C–H_3 Lignin (1465)	0.03	-0.02	0.31	-	0.48	-
1511	C–C stretching of the aromatic ring Lignin (1510)	-0.05	-0.03	0.29	-0.15	0.29	-
1616	C=C Lignin (1595)	0.18	0.06	-	-	0.45	-
2919	C-H stretching Cellulose I (2900) Cellulose II (2900)	0.02	0.03	0.21	0.40	0.58	0.24
3400	–OH stretching intramolecular hydrogen bonds Cellulose I (3352) Cellulose II (3447)	-0.01	-0.02	-0.6	0.09	0.06	0.09

*Au: Autohydrolysis

Table S5: The percentage of glucan, hemicellulose, and lignin content of poplar wood, pine wood, and rice straw

Substrate	Pretreatment Type	Glucan (%)	Hemicellulosic sugar (%)	Lignin (%)	Lignin and hemicellulose removal (%)
Poplar	Untreated	51.4	24.6	25.1	-
	Autohydrolysis	57.8	12.9	27.8	8.9
	Sulfuric Acid	64.1	6.6	32.9	10.1
	Phosphoric Acid	61.2	8.0	23.0	18.7
	Hot Sodium Hydroxide	65.3	13.0	23.2	13.4
	Cold Sodium Hydroxide	55.4	13.7	23.8	12.2
	Sodium Carbonate	52.0	14.0	23.3	12.4
Pine	Untreated	44.2	19.1	23.1	-
	Autohydrolysis	51.8	9.4	21.9	10.9
	Sulfuric Acid	52.7	7.0	29.2	6.0
	Phosphoric Acid	47.4	8.0	27.4	6.9
	Hot Sodium Hydroxide	47.0	12.5	25.5	4.2
	Cold Sodium Hydroxide	45.9	12.7	22.4	7.1
	Sodium Carbonate	48.6	11.4	27.9	2.9
Rice Straw	Untreated	41.8	21.9	20.0	-
	Autohydrolysis	52.7	13.2	18.4	10.3
	Sulfuric Acid	59.8	7.1	19.4	15.4
	Phosphoric Acid	63.0	8.5	19.4	14.0
	Hot Sodium Hydroxide	71.2	11.1	9.7	21.0
	Cold Sodium Hydroxide	60.5	12.8	15.3	13.8
	Sodium Carbonate	57.8	14.2	10.7	17.0