Supplementary Information

One-pot lignocellulose fractionation towards efficient whole sugars conversion and aromatic monomers production by mild alkaline oxidation system

Ziyi Yang[ab1], Feiyue Shen[ab1], Weihong Dai[ab], Zhiwen Zeng[ab], Jiayi Xu [ab], Li Zhao[ab], Wei Qi[c], Jinguang Hu[d], Dong Tian[ab] and Fei Shen[ab, *]

a. College of Environmental Sciences, Sichuan Agricultural University, Chengdu, Sichuan 611130, PR China

b. Sichuan Provincial Engineering Research Center of Agricultural Non-point Source Pollution Control, Sichuan Agricultural University, Chengdu, Sichuan 611130, PR China

c. Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, Guangzhou 510640, China

d. Department of Chemical and Petroleum Engineering, University of Calgary, 2500 University Dr. NW, Calgary, AB T2N 1N4, Canada

* Corresponding author

Fei Shen, E-mail: fishen@sicau.edu.cn. Tel: +86-28-86293087

[1] These authors contributed equally to the work.

Content list:

Table S1. Assignment of main ^{13}C-^{1}H cross-signals in HSQC spectra of these lignin samples.

Labels	δ_C/δ_H (ppm)	Assignment
B_β	53.5/3.06	C_β–H_β in β-β (resinol) substructures (B)
Methoxyl	55.6/3.73	C−H in methoxyls
A_γ	59.5/3.20−3.63	C_γ–H_γ in β-O-4 substructures (A)
A'_γ	63.0/4.36	C_γ–H_γ in β-O-4 substructures (A′)
C_γ	62.5/3.73	C_γ–H_γ in phenylcoumaran substructures (C)
B_γ	71.0/3.82−4.18	C_γ–H_γ in β-β (resinol) substructures (B)
B_α	84.8/4.65	C_α–H_α in β-β (resinol) substructures (B)
A_α	71.8/4.86	C_α–H_α in β-O-4 linked to S units (A)
$A_{\beta(G)}$	83.9/4.29	C_β–H_β in β-O-4 substructures linked to G and H units (A)
$A_{\beta(S)}$	85.9/4.12	C_β–H_β in β-O-4 substructures linked to S units (A)
C_α	86.8/5.46	C_α–H_α in phenylcoumaran substructures (C)
$S_{2,6}$	103.8/6.71	$C_{2,6}$–$H_{2,6}$ in etherified syringyl units (S)
G_2	110.9/6.98	C_2–H_2 in guaiacyl units (G)
PCE_8	114.2/6.27	C_8–H_8 in p-coumarate (PCE)
G_5	114.9/6.77	C_5–H_5 in guaiacyl units (G)
G_6	119.0/6.80	C_6–H_6 in guaiacyl units (G)
$H_{2,6}$	127.9/7.19	$C_{2,6}$–$H_{2,6}$ in p-hydroxyphenyl units (H)
$PCE_{2,6}$	131.2/7.45	$C_{2,6}$–$H_{2,6}$ in p-coumarate (PCE)
PCE_7	144.8/7.51	C_7–H_7 in p-coumarate (PCE)
FA_2	110.7/7.35	C_2–H_2 in ferulate (FA)
FA_6	123.1/7.20	C_6–H_6 in ferulate(FA)
CH_3	15.3/1	CH_3 in aliphatic chain
CH_2	25.8/1.5	CH_2 in aliphatic chain (-CH_2-CH_2-CH_3)

Table S2. Residual carbohydrates content in various lignin samples.

	Glucose mg/g	Xylose mg/g
MWL	9.92	2.74
20°C	10.88	6.51
40°C	1.89	2.83
60°C	1.86	2.38
80°C	3.00	2.88
10%	2.63	4.71
20%	1.61	2.92
30%	3.17	3.64
40%	3.01	3.35

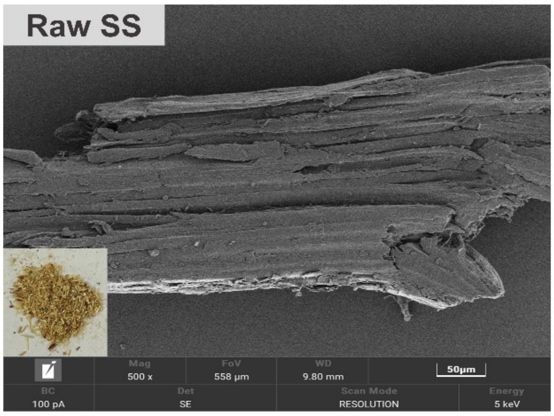

Fig. S1. SEM image of raw sorghum straw.

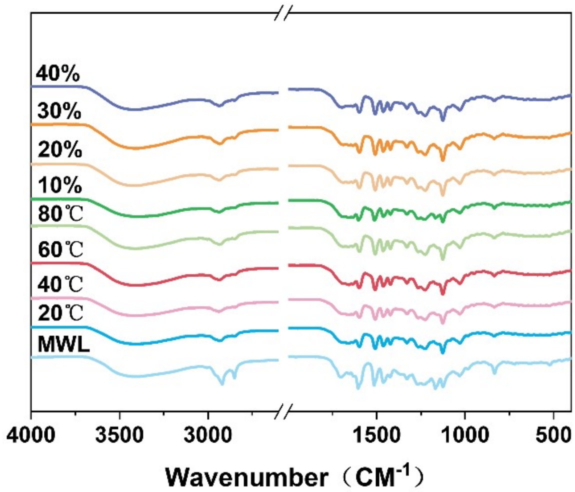

Fig. S2. FTIR spectra of MWL and extracted lignin samples.

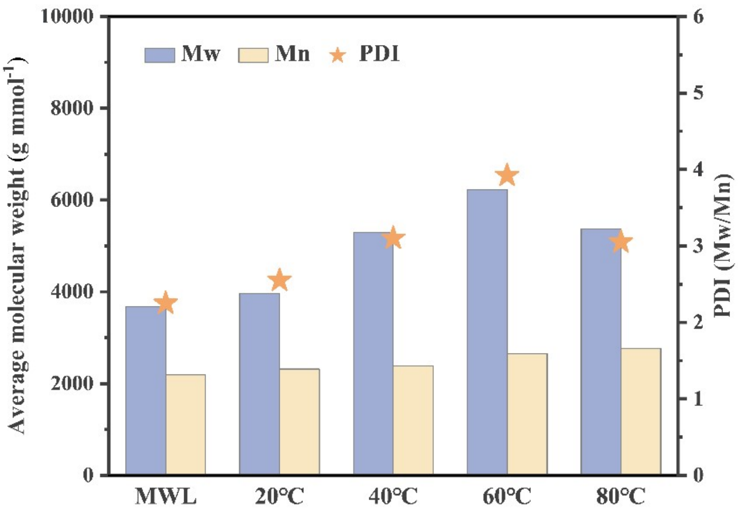

Fig. S3. Average molecular weights and polydispersity index (PDI) of the TMAH/UHP extracted lignin and MWL.

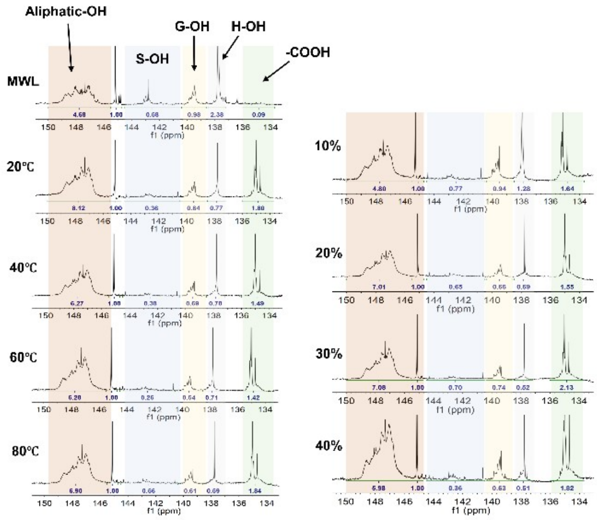

Fig. S4. Quantitative 31^{P} NMR spectra of MWL and extracted lignin samples.

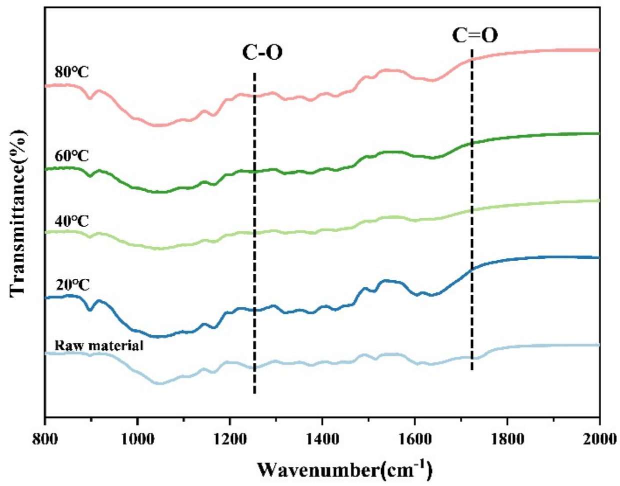

Fig. S5. Growth status of corn seed under different fertilization treatments (a) on the third day, (b) on the tenth day.

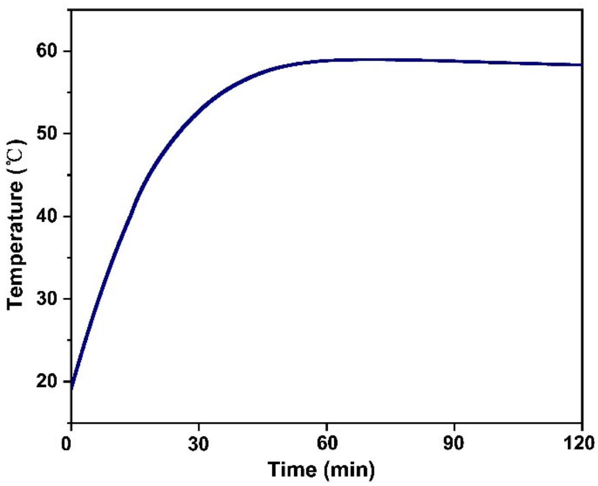

Fig. S6. The self-heating curve of TMAH/UHP reaction at 60 °C.

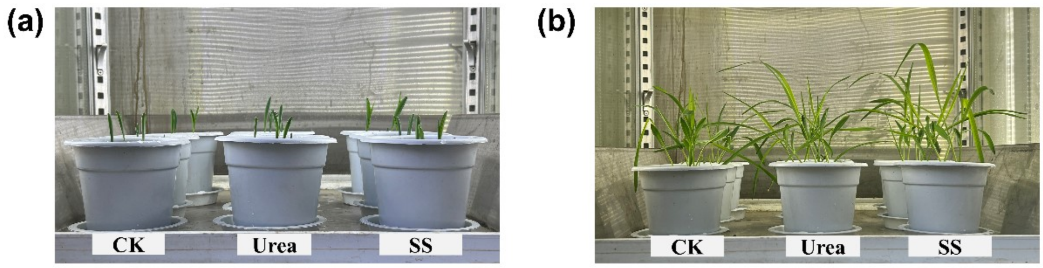

Fig. S7. Growth status of corn seed under different fertilization treatments (a) on the third day, (b) on the tenth day.