

Supplement Table 1 Detailed assignments of ^{13}C - ^1H correlation signals in the HQSC for kraft lignin

Lable	$\delta_{\text{C}}/\delta_{\text{H}}$ (ppm)	Assignments
C_{β}	53.5/3.4	C_{β} - H_{β} in phenylcoumaran substructures
B_{β}	54.1/3.06	C_{β} - H_{β} in β - β (resinol) (B)
A_{γ}	58-61/3.1-3.7	C_{γ} - H_{γ} in β -O-4 substructures (A)
C_{γ}	63.5/3.8	C_{γ} - H_{γ} in phenylcoumaran substructures
B_{γ}	71.4-71.5/3.7-4.2	C_{γ} - H_{γ} in β - β (resinol) (B)
A_{α}	72.5/4.87	C_{α} - H_{α} in α -O-4 substructures linked to a S unit (A)
$\text{A}_{\beta}(\text{G}/\text{H})$	81.9/4.76	C_{β} - H_{β} in β -O-4 substructures linked to a G unit (A)
B_{α}	85.7/4.62	C_{α} - H_{α} in β - β (resinol) substructures (B)
$\text{A}_{\beta}(\text{S})$	86.5/4.12	C_{β} - H_{β} in β -O-4 substructures linked to S
$\text{S}_{2,6}$	105.5/6.52	$\text{C}_{2,6}$ - $\text{H}_{2,6}$ in syringyl units (S)
$\text{S}'_{2,6}$	107.6/6.77	$\text{C}_{2,6}$ - $\text{H}_{2,6}$ in oxidized ($\text{C}\alpha\text{OOH}$) syringyl units (S')
FA2	110.2/7.14	C_2 - H_2 in ferulate
G_2	112.8/6.85	C_2 - H_2 in guaiacyl units (G)
G_5	116.0/6.76	C_5 - H_5 in guaiacyl units (G)
G_6	119.8/6.94	C_6 - H_6 in guaiacyl units (G)
$\text{H}_{2,6}$	126-127/7.2-7.3	$\text{C}_{2,6}$ - $\text{H}_{2,6}$ in p-hydroxyphenyl units (H)
X_2	73.1/3.06	C_2 - H_2 in β -D-xylopyranoside
X_3	74.4/3.26	C_3 - H_3 in β -D-xylopyranoside
X_4	75.9/3.52	C_4 - H_4 in β -D-xylopyranoside
X_5	63.3/3.40	C_5 - H_5 in β -D-xylopyranoside

Supplement Table 2 Quantified yield of monophenols from kraft lignin catalytic pyrolysis under different reaction regimes

Compounds	Yield (wt %)							
	N ₂				H ₂ /N ₂ =1/9			
	Blank	NiO	Co ₃ O ₄	MoO ₂	Blank	NiO	Co ₃ O ₄	MoO ₂
2-methoxy-Phenol	0.56	0.44	0.51	0.43	0.42	0.45	0.37	0.57
2-methoxy-4-methyl-Phenol	0.65	0.50	0.63	0.54	0.48	0.52	0.43	0.70
4-ethyl-2-methoxy-Phenol	0.31	0.24	0.28	0.24	0.21	0.23	0.18	0.29
2,6-dimethoxy-Phenol	2.56	2.06	2.42	2.19	1.94	1.98	1.62	2.76
Total	4.08	3.24	3.84	3.40	3.05	3.18	2.60	4.32