

Flowthrough Pretreatment of Softwood under Water-only and Alkali Conditions

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Supplementary Materials

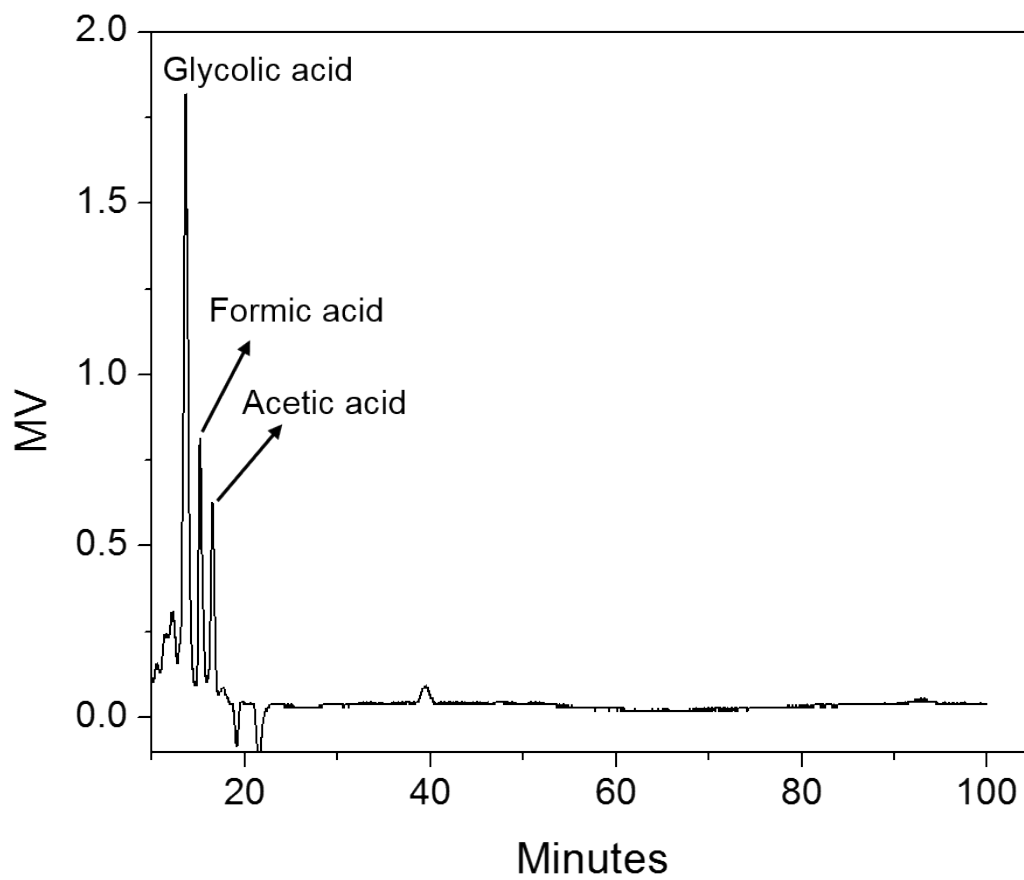
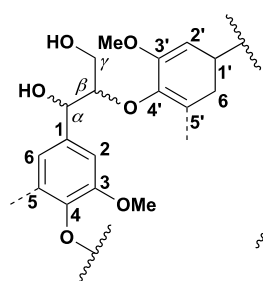
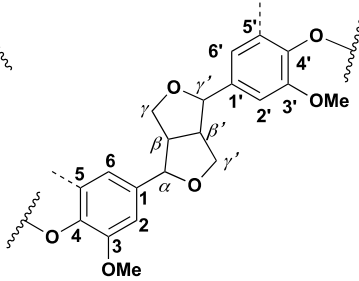


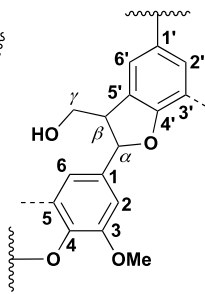
Figure S1. HPLC analysis of degradation products in pretreatment hydrolysates at pH of 12.0 and pretreatment severity of 6.1.



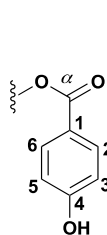
A: β Aryl ether (β -O-4')



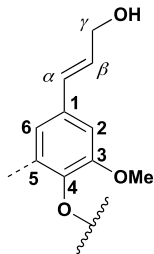
B: resinol (β - β')



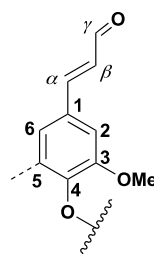
C: phenylcoumaran (β -5')



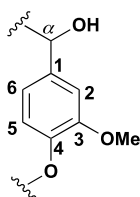
E: *p*-hydroxybenzoate



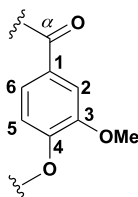
F: *p*-hydroxycinnamyl alcohol end-groups



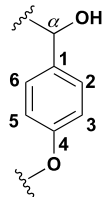
K: cinnamyl aldehyde end-groups



G: guaiacyl units



G': oxidized ($C_{\alpha}=O$) guaiacyl units



H: *p*-hydroxyphenyl units

Figure S2. Main detected lignin linkages.

Table S1. Main lignin 2D ^1H - ^{13}C cross-peak assignments in the HSQC spectra.

Label	δ_{H} (ppm)	δ_{C} (ppm)	Assignment
-OCH ₃	3.73	56.0	C-H in methoxyls
A _{α}	4.71	71.3	C _{α} -H _{α} in β -O-4' substructures (A)
A _{γ}	3.39-3.42	60.3-60.5	C _{γ} -H _{γ} in β -O-4' substructures (A)
A _{β(G/H)}	4.29	84.0	C _{β} -H _{β} in β -O-4' substructures linked to G and H units (A)
A _{β(S)}	4.22	84.8	C _{β} -H _{β} in β -O-4' substructures linked to S units (A)
B _{α}	4.65	85.4	C _{α} -H _{α} in resinol (β - β') substructures (B)
B _{β}	3.05	54.0	C _{β} -H _{β} in resinol (β - β') substructures (B)
B _{γ}	3.80 and 4.16	71.6	C _{γ} -H _{γ} in resinol (β - β') substructures (B)
C _{α}	5.43	87.4	C _{α} -H _{α} in phenylcoumaran substructures (C)
C _{β}	3.43	53.6	C _{β} -H _{β} in phenylcoumaran substructures (C)
C _{γ}	3.68	63.1	C _{γ} -H _{γ} in phenylcoumaran substructures (C)
E _{2/6}	7.67	131.8	C _{2,6} -H _{2,6} in <i>p</i> -hydroxybenzoate substructures (E)
F _{γ}	4.09	61.9	C _{γ} -H _{γ} in <i>p</i> -hydroxycinnamyl alcohol end-groups (F)
G ₂	6.97	111.5	C ₂ -H ₂ in guaiacyl units (G)
G ₅	6.74	115.5	C ₅ -H ₅ in guaiacyl units (G)
G ₆	6.76	119.1	C ₆ -H ₆ in guaiacyl units (G)
G' ₂	7.38	111.0	C ₂ -H ₂ in oxidized (C _{α} =O) guaiacyl units (G')
G' ₆	7.5	123.4	C ₆ -H ₆ in oxidized (C _{α} =O) guaiacyl units (G')
H _{2/6}	7.18	128.3	C _{2,6} -H _{2,6} in <i>p</i> -hydroxyphenyl units (H)
K _{β}	6.77	126.7	C _{β} -H _{β} in cinnamyl aldehyde end-groups (K)
X ₂	3.02	73.0	C ₂ -H ₂ in β -D-xylopyranoside
X ₃	3.23	74.4	C ₃ -H ₃ in β -D-xylopyranoside
X ₄	3.49	75.8	C ₄ -H ₄ in β -D-xylopyranoside
X ₅	3.16	63.5	C ₅ -H ₅ in β -D-xylopyranoside
X ₂ ₂	4.49	73.7	C ₂ -H ₂ in 2-O-acetyl- β -D-xylopyranoside
X ₃ ₃	4.78	75.3	C ₃ -H ₃ in 3-O-acetyl- β -D-xylopyranoside