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Natural deep eutectic solvent mediated extrusion for continuous high-solid pretreatment of lignocellulosic biomass

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Labels	δ _C /δ _H (ppm)	Assignment
Β _β	53.2/3.47	C_{β}/H_{β} in β -5' phenylcoumaran substructures (B)
C _β	53.6/3.06	C_{β}/H_{β} in β - β ' resinol substructures (C)
OMe	55.5/3.71	C/H in methoxyls
\mathbf{A}_{γ}	59.8/3.36 & 3.58	C_{γ}/H_{γ} in normal (γ -hydroxylated) β -O-4' substructures (A)
I_{γ}	61.4/4.08	C_{γ}/H_{γ} in cinnamyl alcohol end-groups (I)
\mathbf{B}_{γ}	62.5/3.75	C_{γ}/H_{γ} in β -5' phenylcoumaran substructures (B)
I'γ	64.1/4.70	C_{γ}/H_{γ} in γ -acylated cinnamyl alcohol end-groups (I')
A'γ	62.8/3.70	C_{γ}/H_{γ} in γ -acylated β -O-4' substructures (A')
HKα	85.2/4.63	C_{α}/H_{α} in Hibbert ketone (HK)
Cγ	71.2/3.80 &4.17	C_{γ}/H_{γ} in β - β ' resinol substructures (C)
A_{α}/A'_{α}	71.5/4.75& 71.9/4.89	C_{α}/H_{α} in β -O-4' substructures (A, A') -G&-S, respectively
$A'_{\beta(G)}$	83.0/4.23	C_{β}/H_{β} in γ -acylated β -O-4' substructures linked to a G unit (A')
$A'_{\beta(S)}$	83.3/4.33	C_{β}/H_{β} in γ -acylated β -O-4' substructures linked to an S unit (A')
$A_{\beta(G)}$	83.4/4.31	C_{β}/H_{β} in β -O-4' substructures linked to a G unit (A)
Cα	85.2/4.63	C_{α}/H_{α} in β - β ' resinol substructures (C)
$A_{\beta(S)}$	85.8/4.09	C_{β}/H_{β} in β -O-4' substructures linked to an S unit (A)
B _α	87.0/5.46	C_{α}/H_{α} in β -5' phenylcoumaran substructures (B)
T ₈	94.3/6.56	C_8/H_8 in tricin units (T)
T ₆	99.0/6.22	C_6/H_6 in tricin units (T)
S _{2/6}	103.9/6.65	C_2/H_2 and C_6/H_6 in etherified syringyl units (S)
T _{2'/6} ,	104.1/7.29	$C_{2'}/H_{2'}$ and $C_{6'}/H_{6'}$ in tricin units (T)
T ₃	104.9/7.03	C_3/H_3 in tricin units (T)
S' _{2/6}	106.4/7.26	C_2/H_2 and C_6/H_6 in α -oxidized syringyl units (S')
G ₂	110.9/6.95	C_2/H_2 in guaiacyl units (G)
FA ₂	111.0/7.30	C_2/H_2 in ferulic acid units (FA)
G' ₂	112.5/7.29	C_2/H_2 in in α -oxidized guaiacyl units (G')
pCA _β	113.7/6.28	C_{β}/H_{β} in <i>p</i> -coumarate (<i>p</i> CA)
FAβ	113.7/6.28	C_{β}/H_{β} in <i>p</i> -ferulate (FA)
H _{3/5}	114.5/6.63	C_3/H_3 and C_5/H_5 in <i>p</i> -hydroxyphenyl units (H)
G ₅	115.1/6.75 & 6.98	C_5/H_5 in guaiacyl units (G)
G ₆	118.8/6.78	C_6/H_6 in guaiacyl units (G)
I'β	123.5/6.40	C_{β}/H_{β} in γ -acylated cinnamyl alcohol end-groups (I')
$H_{2/6}$	127.9/7.21	C_2/H_2 and C_6/H_6 in <i>p</i> -hydroxyphenyl units (H)
I _β	128.8/6.21	C_{β}/H_{β} in cinnamyl alcohol end-groups (I)
<i>p</i> CA _{2/6}	130.0/7.22	C_2/H_2 and C_6/H_6 in <i>p</i> -coumarate (<i>p</i> CA)
pCA _α	144.8/7.22-7.52	C_{α}/H_{α} in <i>p</i> -coumarate (<i>p</i> CA)
FA_{α}	144.8/7.22-7.52	C_{α}/H_{α} in <i>p</i> -ferulate (FA)

Table **S1** Assignments of the lignin ¹³C–¹H correlation signals observed in the HSQC spectra of the sorghum lignins ¹⁻³

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