

Supporting Information

Structural Characterization and Antioxidant Activity of Milled Wood Lignin from Xylose Residue and Corncob

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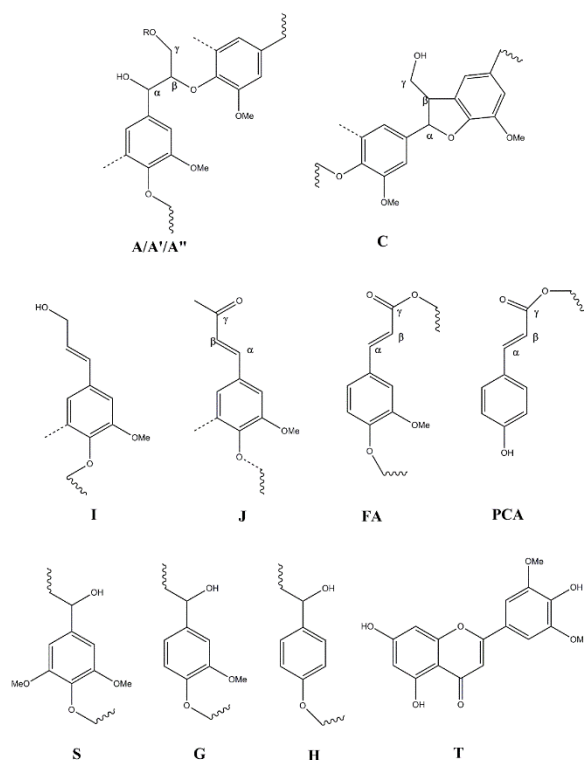


Figure S1. Main structures of lignin fractions of corn cob, involving different side-chain linkages, and aromatic units by 2D HSQC NMR. (A) β -O-4' linkages; (A') β -O-4 linkages with acetylated γ -carbon; (A'') β -O-4 linkages with p-coumaroylated γ -carbon; (C) phenylcoumarane structures formed by β -5' and α -O-4' linkages; (I) cinnamyl alcohol end-groups; (J) cinnamyl aldehyde end-groups; (S) syringyl unit; (G) guaiacyl unit; (H) p-hydroxyphenyl unit; (FA) ferulate; (pCA) p-coumarate; (T) tricin.

Table S1. Assignments of main lignin ^{13}C - ^1H correlation signals in the HSQC NMR spectra shown in Figure 2.

Label	$\delta\text{C}/\delta\text{H}$	assignment
A_γ	59.65/3.61 and 3.27	C_γ - H_γ in β -O-4' substructures (A)
I_γ	61.3/4.09	C_γ - H_γ in <i>p</i> -hydroxycinnamyl (sinapyl/coniferyl) alcohol (I)
A'_γ/A''_γ	62.7/3.83-4.30	C_γ - H_γ in γ -acylated β -O-4' substructures (A'/A'')
I'_γ	64.0/4.79	C_γ - H_γ in γ -acylated cinnamyl alcohol end-groups (I')
$A\alpha$	71.8/4.80	$C\alpha$ - $C\alpha$ in β -O-4' substructures
$A_{\beta(G)}$ and $A'_{\beta(S)}$	83.4/4.31	C_β - H_β in β -O-4' substructures linked to a G unit (A) and in γ -acylated β -O-4' substructures linked to a S unit (A')
$A_{\beta(S)}$	85.9/4.12	C_β - H_β in β -O-4' substructures linked to a S unit (erythro) (A)
$S_{2,6}$	103.7/6.71	$C_{2,6}$ - $H_{2,6}$ in etherified syringyl units (S)
$T'_{2,6}$	103.9/7.30	$C_{2',6'}$ - $H_{2',6'}$ in triclin (T)
T_3	104.7/7.03	C_3 - H_3 in triclin (T)
G_2	110.7/6.98	C_2 - H_2 in guaiacyl units (G)
FA_2	111.0/7.32	C_2 - H_2 in ferulate (FA)
$J_{2(G)}$	112.24/7.25	C_2 - H_2 in cinnamyl aldehyde end-groups (J)
pCA_β and FA_β	113.5/6.27	C_β - H_β in <i>p</i> -coumarate (<i>pCA</i>) and ferulate (FA)
G_5	114.9/6.72 and 6.94	C_5 - H_5 in guaiacyl units (G)
$PCA_{3,5}$	115.5/6.77	$C_{3,5}$ - $H_{3,5}$ in <i>p</i> -coumarate (<i>pCA</i>)
G_6	118.7/6.77	C_6 - H_6 in guaiacyl units (G)
$J_{6(G)}$	122.3/7.10	C_6 - H_6 in cinnamyl aldehyde end-groups (J)
$H_{2,6}$	127.8/7.22	$C_{2,6}$ - $H_{2,6}$ in <i>p</i> -hydroxyphenyl units (H)
$PCA_{2,6}$	129.9/7.46	$C_{2,6}$ - $H_{2,6}$ in <i>p</i> -coumarate (<i>pCA</i>)
PCA_α and FA_α	144.7/7.45	C_α - H_α in <i>p</i> -coumarate (<i>pCA</i>) and ferulate (FA)