Supplementary information for:

Catalytic hydrotreatment of Alcell lignin fractions using a Ru/C catalyst

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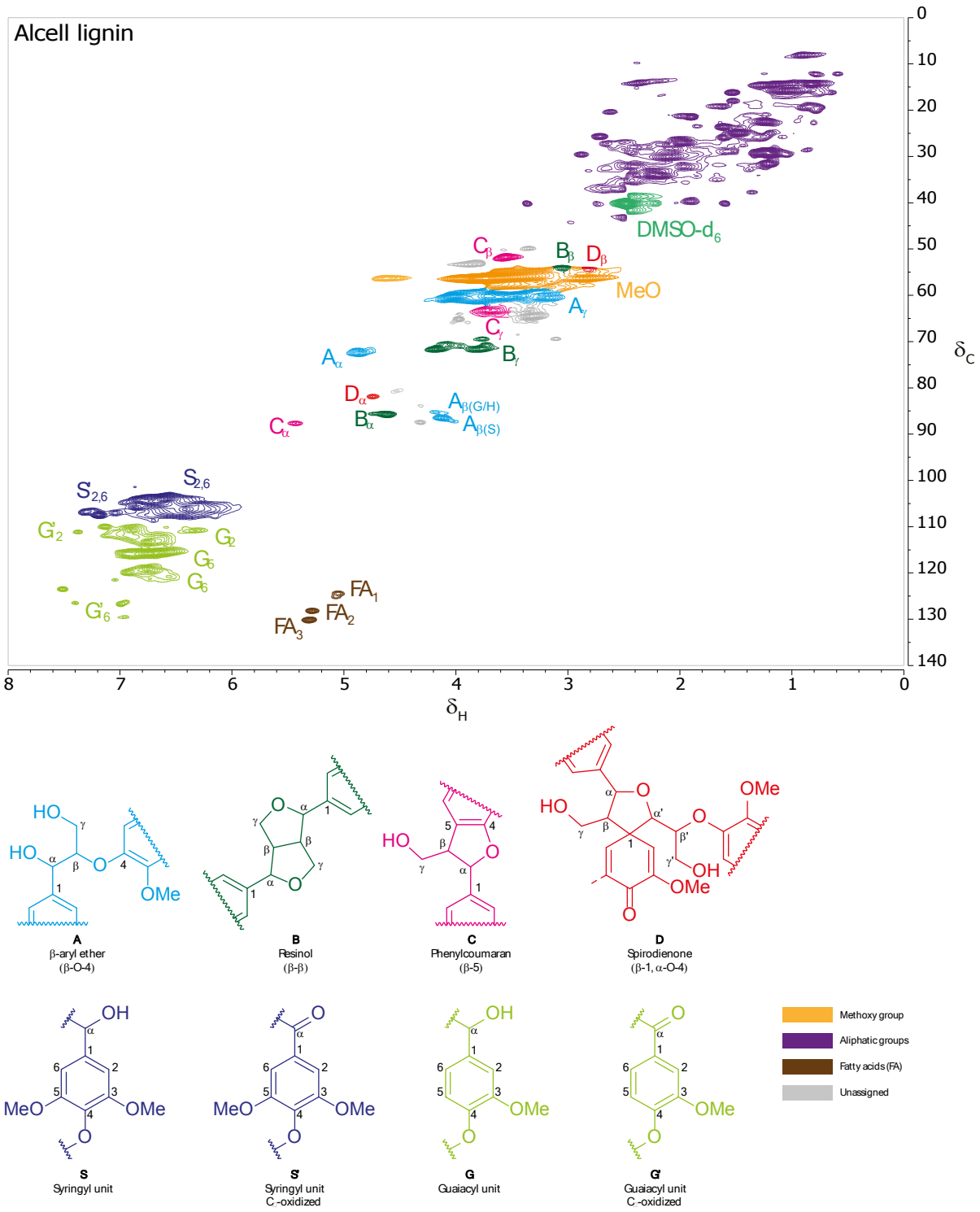
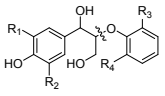
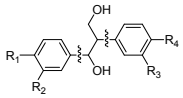
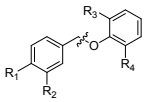
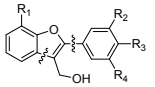
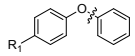
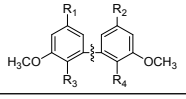


Figure S1. Full HSQC (δ_C 0-140, δ_H 0-8 ppm) of Alcell lignin and the fractionated lignins. The contours are colour coded according to the linkage they are assigned to with purple being used for the aliphatic area. Light grey contours are unknown regions.

Table S1. Assignments of ^{13}C-^{1}H cross signals in the gradient HSQC spectra (δ_C 50-90 ppm) of Alcell lignin.

Lable	**δ_C/δ_H (ppm)**	**Assignment**
C_β	53.33/3.49	C_β-H_β in phenylcoumaran (β-5)
B_β	53.33/3.49	C_β-H_β in resinol (β-β)
D_β	54.25/2.84	C_β-H_β in spirodienone substructure (β-1, α-O-4)
OMe	56.17/3.75	C-H in methoxyls (OCH_3)
A_γ	60.0/3.40-3.80	C_γ-H_γ in β-aryl ether (β-O-4)
C_γ	63.2/3.68	C_γ-H_γ in phenylcoumaran (β-5)
B_γ	71.4/3.8-4.2	C_γ-H_γ in resinol (β-β)
A_α	72.4/4.90	C_α-H_α in β-aryl ether (β-O-4)
D_α	81.8/4.76	C_α-H_α in spirodienone substructure (β-1, α-O-4)
$A_{\beta(G/H)}$	72.4/4.90	C_β-H_β in β-aryl ether (β-O-4)
B_α	85.53/4.63	C_α-H_α in resinol (β-β)
$A_{\beta(S)}$	86.3/4.15	C_β-H_β in β-aryl ether (β-O-4)
C_α	87.5/5.44	C_α-H_α in phenylcoumaran (β-5)
$S_{2,6}$	63.9/6.62	$C_{2,6}$-$H_{2,6}$ in syringyl units (S)
$S'_{2,6}$	67.3/7.2	$C_{2,6}$-$H_{2,6}$ in oxidized Cα-oxidized syringyl units (S')
G_2	70.7/6.91	C_2-H_2 in guaiacyl units (G)
G_5	75.6/6.75	C_5-H_5 in guaiacyl units (G)
G_6	79.0/6.75	C_6-H_6 in guaiacyl units (G)
G'_6	83.4/7.5	C_6-H_6 in oxidized Cα-oxidized guaiacyl units (G')
FA_1	84.3/5.07	Unsaturated bonds in fatty acids
FA_2	88.0/5.3	Unsaturated bonds in fatty acids
FA_3	50.0/5.33, 90.0/5.33	Unsaturated bonds in fatty acids
Aliphatic	50-90/3.1-0	Aliphatic chains

Table S2. Bond dissociation enthalpies (BDE) for lignin linkages.

Linkage bond		BDE (KJ/mol)	Linkage bond		BDE (KJ/mol)
	β-O-5	292 ±5[a] 281 ±1[b]		β-1	289 ±2[a]
	α-O-4	220 ±16[a]		β-5	430 ±8[a]
	4-O-5	332 ±7[b]		5-5	482 ±12[a] 488 ±12[b]

a) Calculated BDE values from Parthasarathi et al.[1], b) Calculated BDE values from Kim et al.[2]

References for supplementary information

1 R. Parthasarathi, R. A. Romero, A. Redondo and S. Gnanakaran, *J. Phys. Chem. Lett.,* 2011, **2**, 2660-2666.

2 S. Kim, S. C. Chmely, M. R. Nimos, Y. J. Bomble, T. D. Foust, R. S. Paton and G. T. Beckham, *Journal of Physical Chemistry Letters,* 2011, **2**, 2846-2852.