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Supporting Information for:

Highly efficient catalytic transfer hydrogenolysis for the conversion of Kraft lignin into bio-oil over heteropoly acids

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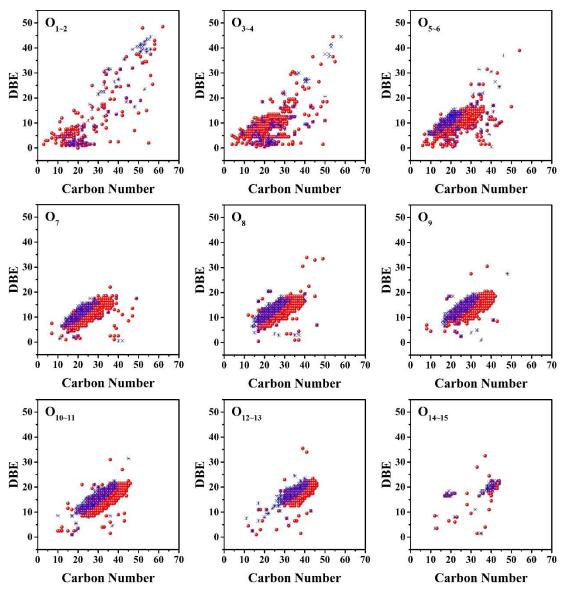


Fig. S1 Double bond equivalent (DBE) vs. carbon number plots for oxygen class compounds in EKL (※) and lignin oil (●), observed with negative-ion ESI.

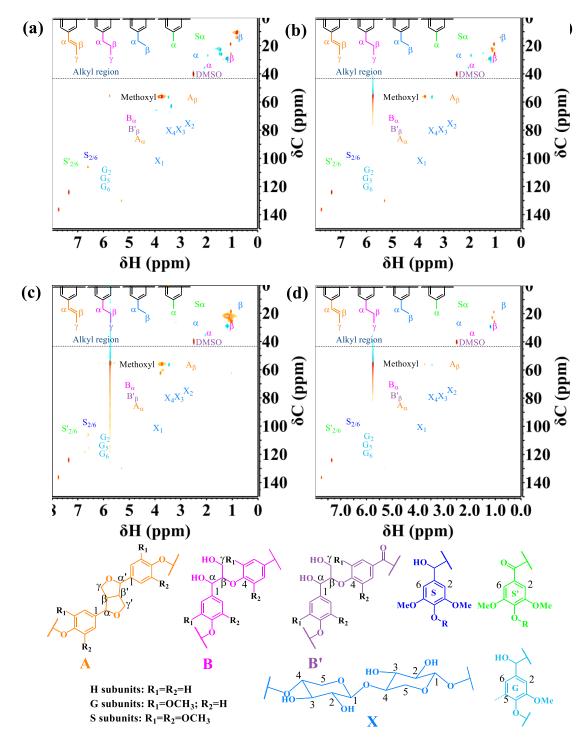


Fig. S2 (a) EKL oil obtained over H₄PW at 190 °C in iso-propanol; (b) EKL oil obtained over H₄SiW at 190 °C in *n*-propanol; (c) EKL oil obtained over H₄SiW at 170 °C in iso-propanol and (d) PKL oil obtained over H₄PW at 190 °C in iso-propanol.

Table S1 Assignments of the main ¹³C-¹H correlation signals in the HSQC spectra^[1]

Labels	Chemical shift	Assignments
	$\delta_C/\delta_H \ (ppm)$	
A_{α}	85.8/4.65	C_{α} -H _{α} in resinol substructures
A_{β}	54.1/3.07	C_{β} -H $_{\beta}$ in resinol substructures
OCH_3	56.2/3.73	C–H in methoxyls
$B_{\boldsymbol{\alpha}}$	71.5/4.75	$C_{\alpha}\text{-}H_{\alpha}$ in $\beta\text{-}O\text{-}4'$ linked to G units
$B_{\boldsymbol{\alpha}}$	72.2/4.98	$C_{\alpha}\text{-}H_{\alpha}$ in $\beta\text{-}O\text{-}4'$ linked to S units
$\mathrm{B}'eta$	81.9.2/4.77	$C_{\beta}\text{-}H_{\beta}$ in $\beta\text{-}O\text{-}4'$ substructures with a conjugated carbonyl
		or carboxyl group
X_1	102.2/4.29	C ₁ -H ₁ in xylan
X_2	73.1/3.14	C ₂ -H ₂ in xylan
X_3	74.6/3.34	C ₃ -H ₃ in xylan
X_4	75.9/3.58	C ₄ -H ₄ in xylan
S _{2,6}	104.0/6.62,	C _{2,6} -H _{2,6} in syringyl units
	6.86	
	105.3/7.00,	
	7.10	
S'2,6	106.6/7.26	$C_{2,6}$ - $H_{2,6}$ in oxidized ($C\alpha$ = O) syringyl units
	107.7/7.22	
	108.5/7.22	
	109.7/7.15	
G_2	112.9/6.80	C ₂ -H ₂ in guaiacyl units
G_5	115.6/6.74	C ₅ -H ₅ in guaiacyl units
G_6	120.2/6.76	C ₆ -H ₆ in guaiacyl units
	121.0/7.23	

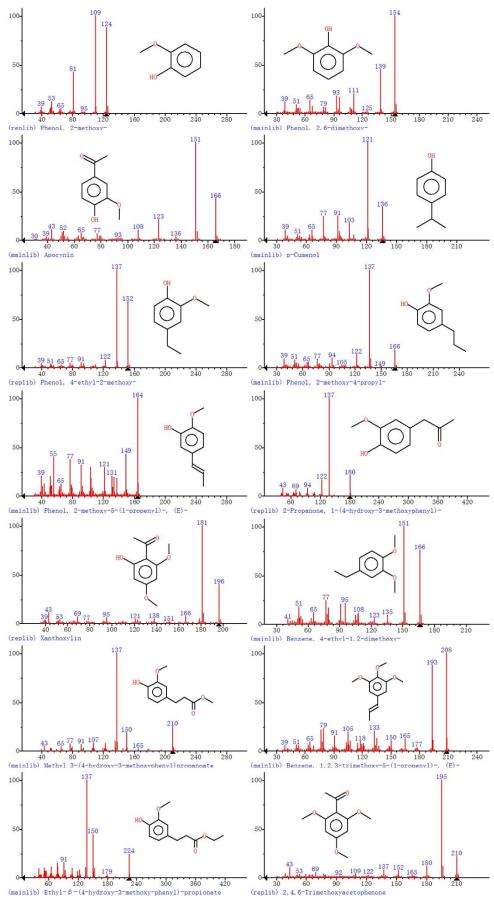


Fig. S3 Mass spectra for the main monomer products from lignin oil

References

[1] a) C. Fernández-Costas, S. Gouveia, M. A. Sanromán, D. Moldes, *Biomass and Bioenergy* **2014**, *63*, 156-166; b) H. Zhang, Y. Bai, B. Yu, X. Liu, F. Chen, *Green Chemistry* **2017**, *19*, 5152-5162.