Electronic Supplementary Material (ESI) for Green Chemistry.

A simple route to synthesize esterified lignin derivatives

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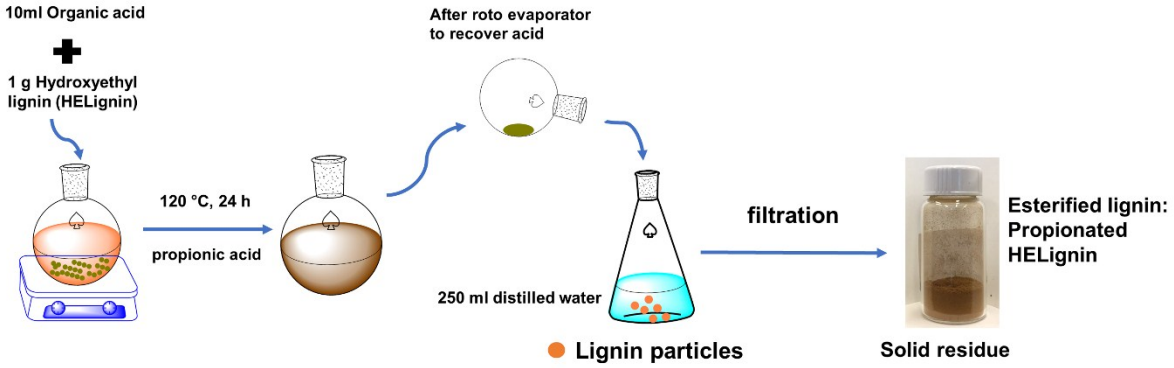


Figure S1 the operating process of direct esterification using propionic acid to obtain propionated HELignin

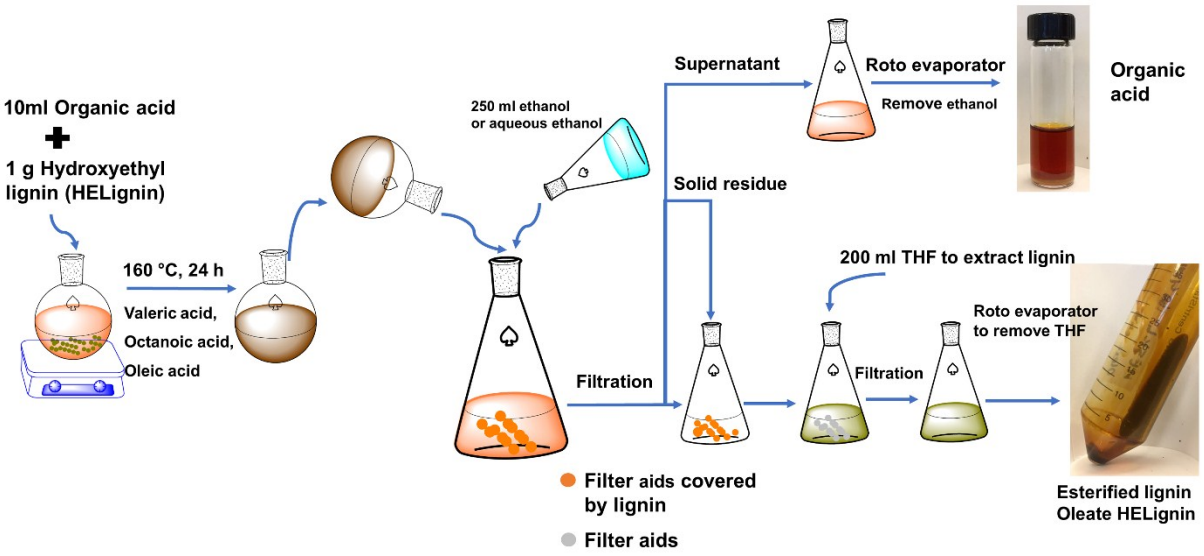


Figure S2 the operating process of direct esterification using valeric acid, octanoic acid, and oleic acid to obtain esterified HELignin

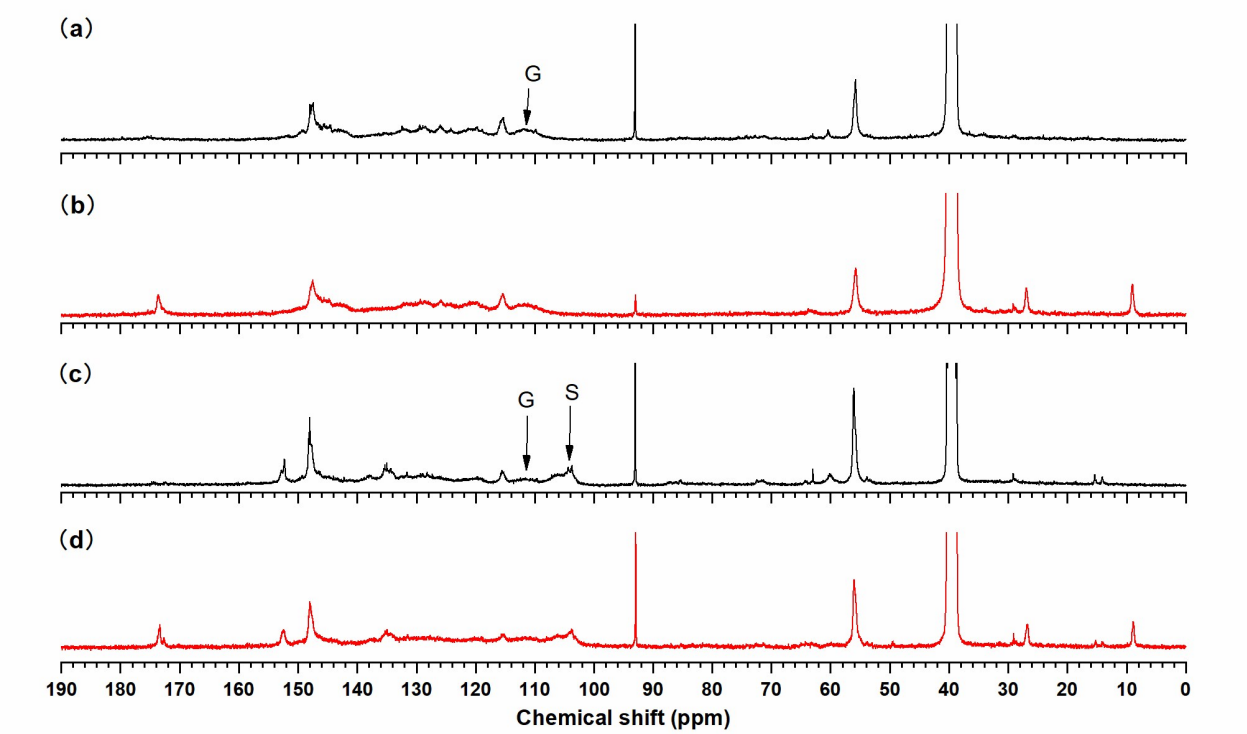


Figure S3 ^{13}C NMR spectrum of SKL (a), propionated SKL (120°C, 24 h, b), OSHL (c), and propionated OSHL (120 °C, 24h, d)

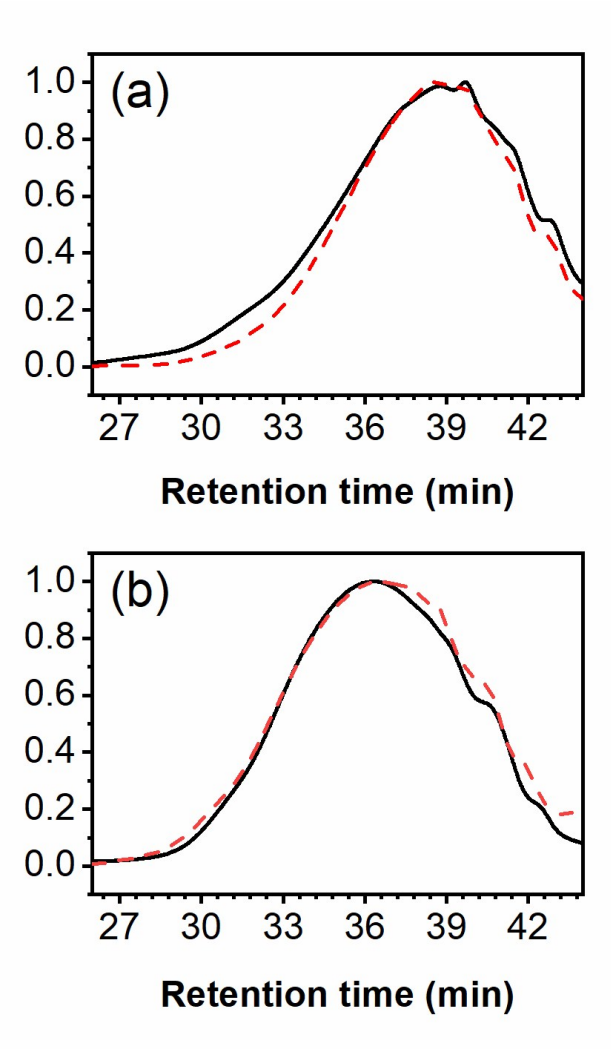


Figure S4 The molecular weight traces of SKL (a) and OSHL before (dark line) and after (red dash) esterification using propionic acid at 120 °C for 24 h

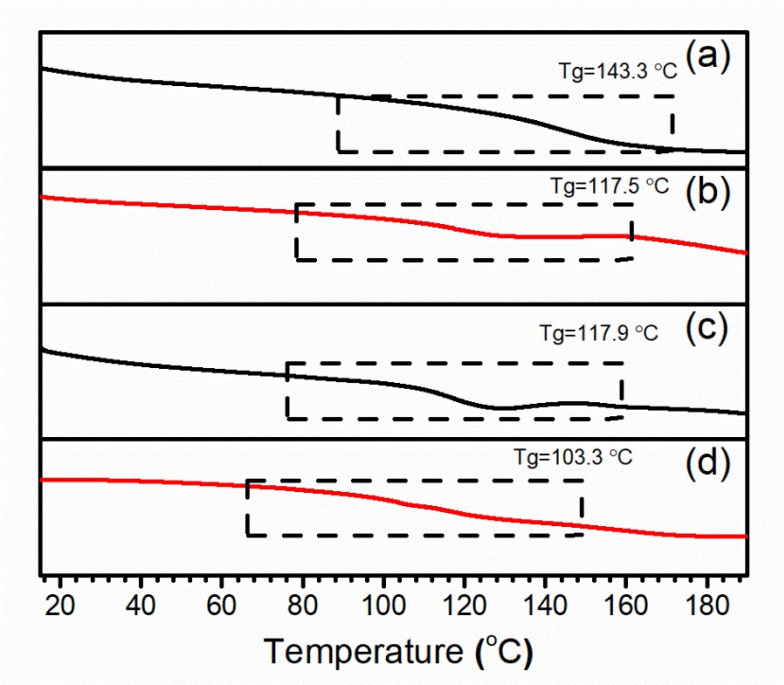


Figure S5 DSC traces and glass transition temperature (T_g) of SKL (a), propionate SKL (b), OSHL (c), and propionate OSHL (d)

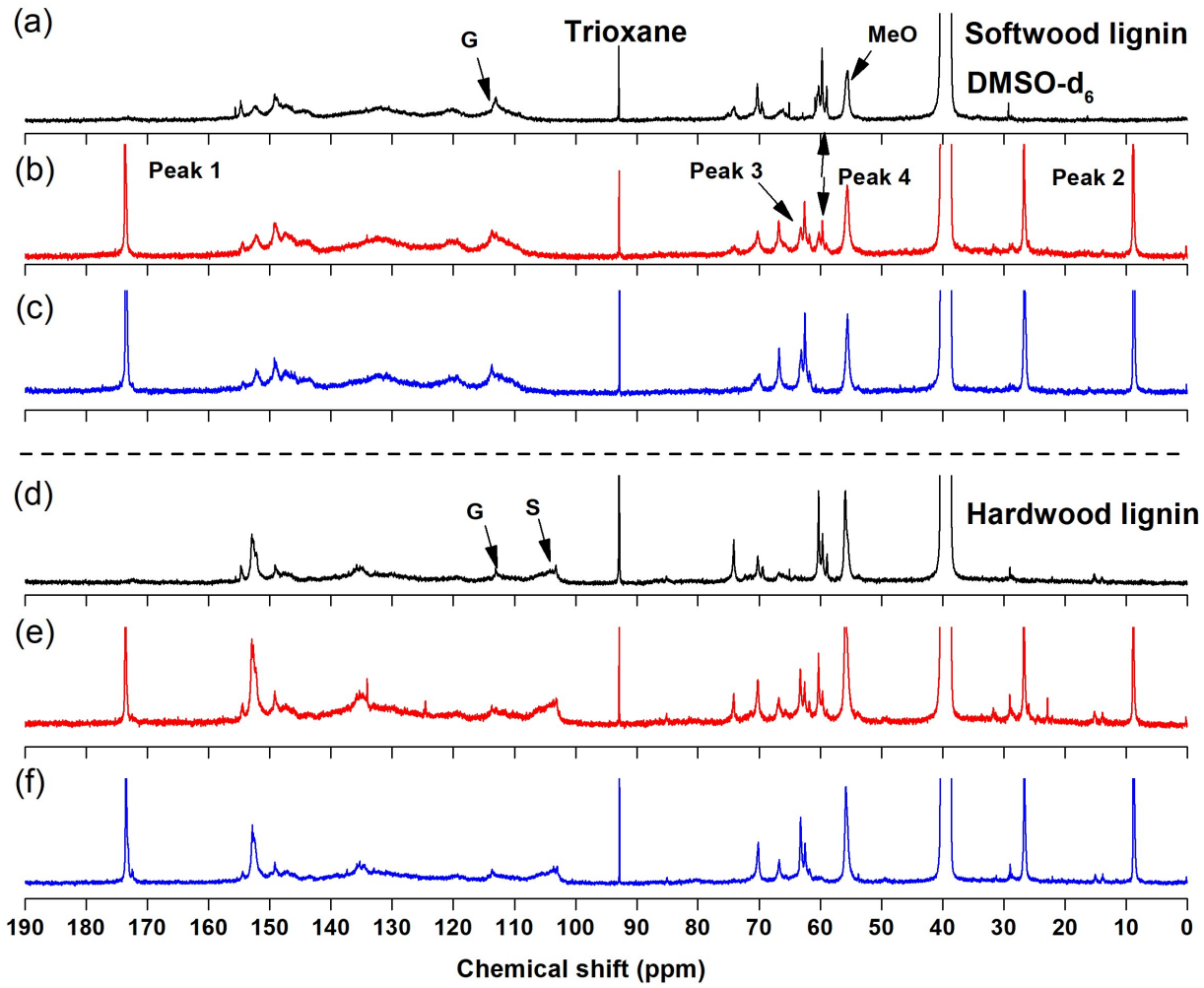


Figure S6 ^{13}C NMR spectrum of HESKL (untreated, a), propionate HESKL (90°C, 24 h, b), propionate HESKL (120 °C, 48 h, c) and HEOSHL (untreated, d), propionate HEOSHL (90°C, 24h, e), and propionate HEOSHL (120 °C, 48 h)

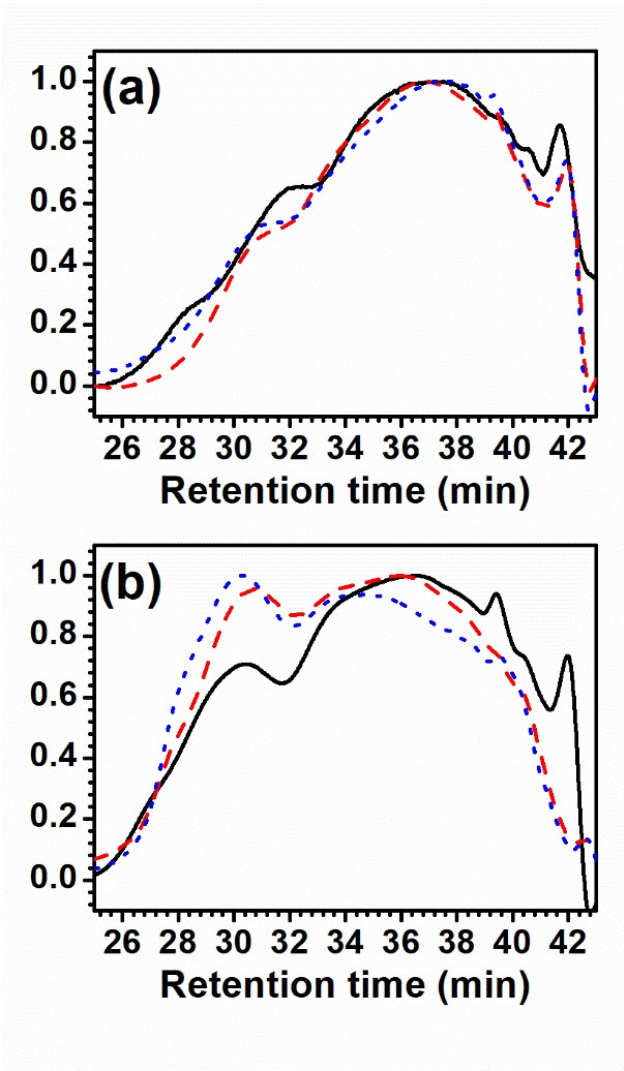


Figure S7 Molecular weight traces of HESKL (a) and HEOSHL (b); (untreated, black line), propionate HELignin (90°C, 24 h, red short dash line), propionate HElignin (120 °C, 48 h, blue dot line)

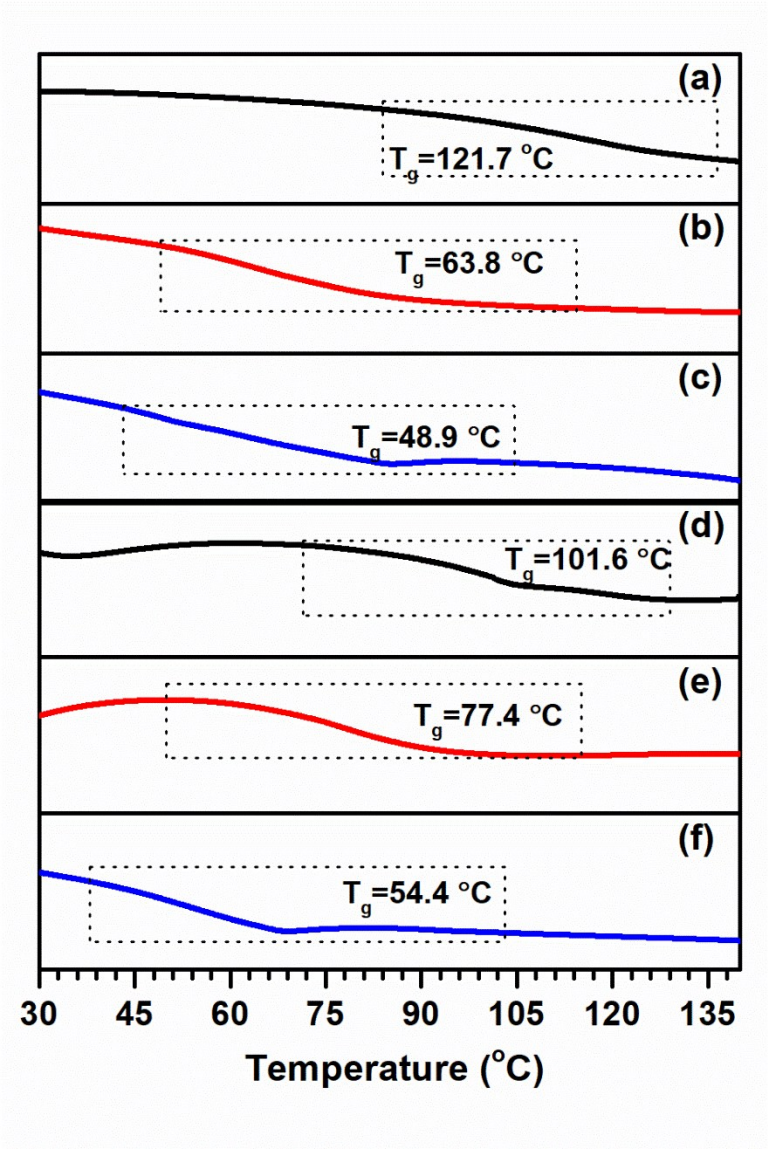


Figure S8 DSC traces and glass transition temperature (T_g) of HESKL (untreated, a), propionate HESKL (90°C, 24 h, b), propionate HESKL (120 °C, 48 h, c) and HEOSHL (untreated, d), propionate HEOSHL (90°C, 24h, e), and propionate HEOSHL (120 °C, 48 h)

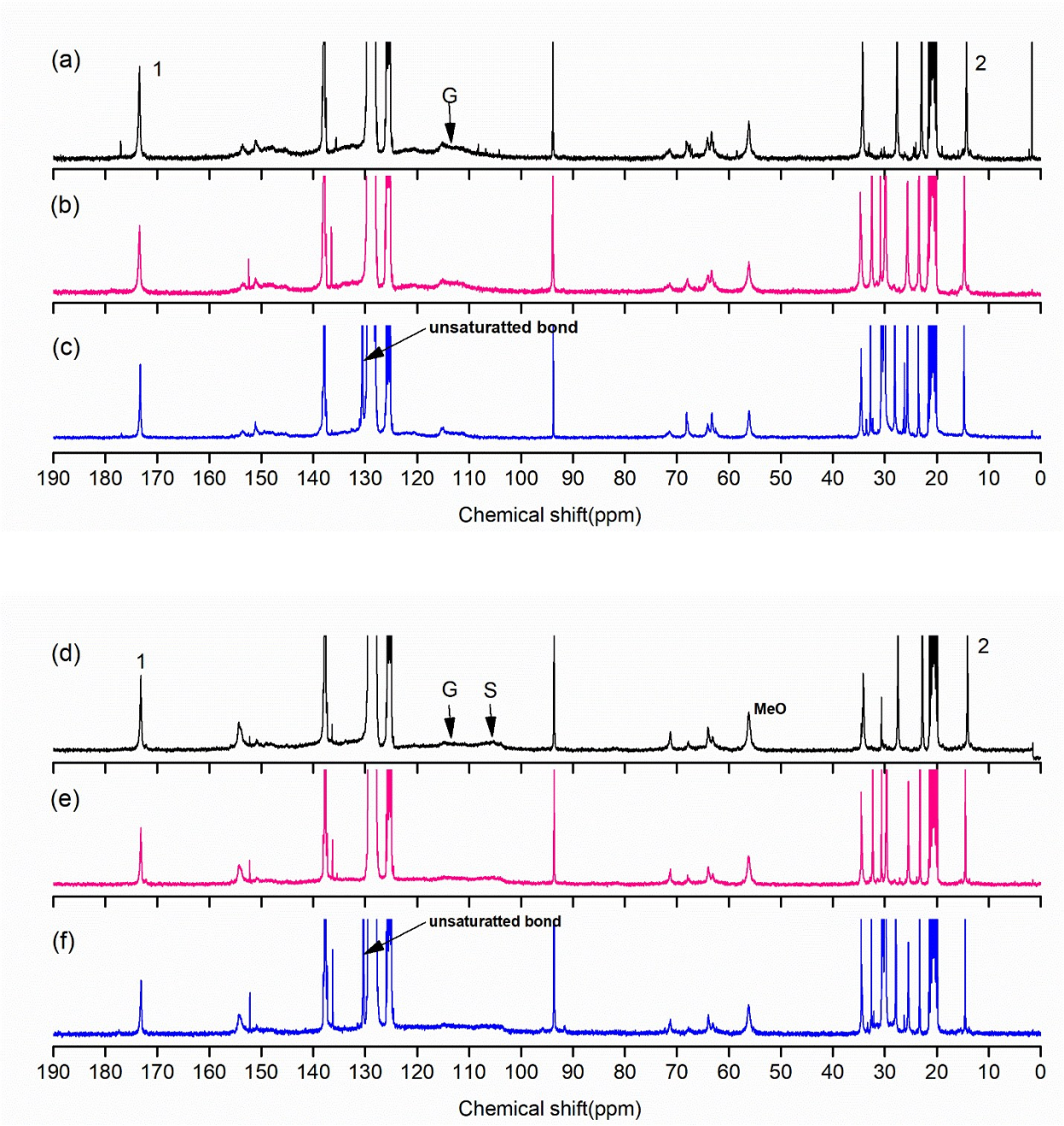


Figure S9 ^{13}C NMR spectrum of valerate lignin HESKL (a), octanoate HESKL (b), oleate HESKL (c) and valerate HEOSHL (d), octanoate HEOSHL (e), and oleate HEOSHL

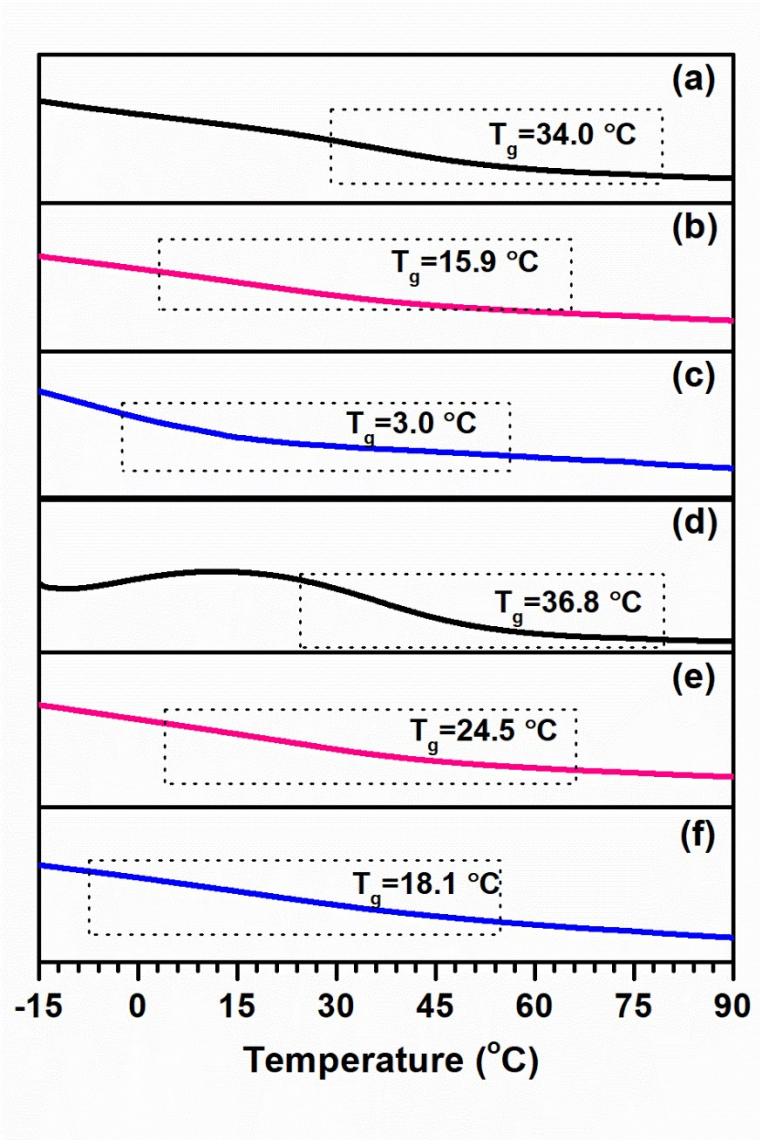


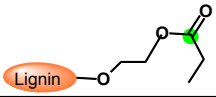
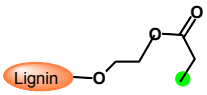
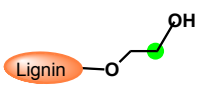
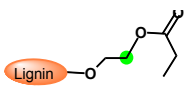
Figure S10 DSC traces and glass transition temperature (T_g) of valerate lignin HESKL (a), octanoate HESKL (b), oleate HESKL (c) and valerate HEOSHL (d), octanoate HEOSHL (e), and oleate HEOSHL

Table S1 Quantitative ^{31}P NMR and semi-quantitative ^{13}C NMR analysis of softwood kraft lignin (SKL), propionate SKL (PSKL), hydroxyethyl SKL (HESKL), organosolv hardwood lignin (OSHL), propionate OSHL (POSHL), and hydroxyethyl OSHL (HEOSHL)

	Syringyl /(mmol/g)	5-substituted /(mmol/g)	Guaiacyl /(mmol/g)	p-hydroxyphenyl /(mmol/g)	Total aromatic OH/(mmol/g)	ArH[a] /(100Ar)
SKL	n.a.	1.68	1.48	0.33	3.49	230
PSKL	n.a.	1.36	1.45	0.24	3.05	231
HESKL	n.a.	0.25	0.14	0.03	0.42	
OSHL	2.34	0.34	1.10	0.29	4.07	201
POSHL	2.08	0.32	0.95	0.25	3.60	201
HEOSHL	0.08	0.08	0.04	0.21	0.41	

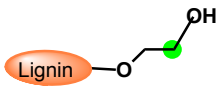
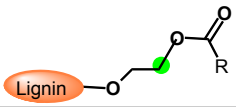
[a] ArH: aromatic carbon linked with hydrogen

Table S2 Semi-quantitative ^{13}C NMR analysis of HELignin and esterified HELignin using propionic acid with different conditions, the aromatic carbon region (160~100 ppm) was set as 100 Ar;

No. Lignin	Temp(°C) /time(h)	Peak 1/100 Ar (175~170 ppm) 	Peak 2/100 Ar (10~8 ppm) 	Peak 3/100 Ar (61.5~58 ppm) 	Peak 4/100Ar (65~61.5 ppm) 	ArH[a]/100Ar (125~100 ppm)
HESKL						
(a)	untreated	-	-	74	14	206
(b)	90/24	57	58	39	54	212
(c)	120/48	82	72	11	72	210
HEOSHL						
(d)	untreated	-	-	72	20	207
(e)	90/24	51	47	43	49	205
(f)	120/48	82	81	19	71	203

[a] ArH: aromatic carbon linked with hydrogen;

Table S3 Semi-quantitative ^{13}C NMR analysis of HELignin and esterified HELignin using valeric acid (C_5), octanoic acid(C_8), and oleic acid (C_{18}), the peak 3 + peak 4 (65~58 ppm) were set as 100,

No.	Lignin	acid	Peak 3 (61.5~58 ppm)/100 Pr 	Peak 4 (65~61.5 ppm)/100 Pr 
	HESKL			
(a)		Valeric (C_5)	17	83
(b)		Octanoic (C_8)	19	81
(c)		Oleic (C_{18})	15	85
	HEOSHL			
(d)		Valeric (C_5)	21	79
(e)		Octanoic (C_8)	19	81
(f)		Oleic (C_{18})	23	77