SUPPORTING INFORMATION

The Effect of Fatty Acid Esterification on the Thermal Properties of Softwood Kraft Lignin

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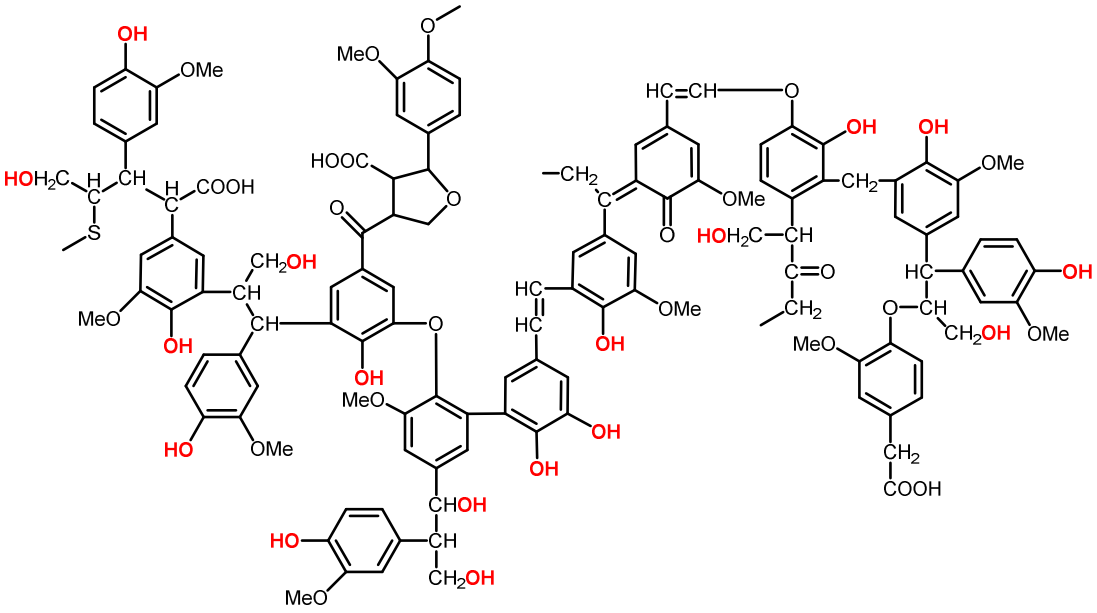

Scheme S1. An early tentative structure of SWKL (Marton 1971).

Hydroxyl group	Amount mmol/g
Aliphatic	**2.3**
Biphenyl	0.9
Diphenylether	0.6
Other condensed	0.7
Total condensed phenolic	**2.1**
Guaiacyl	2.2
p -Hydroxyphenyl	0.1
Total noncondensed phenolic	**2.3**
COOH	0.4
Total OH	**6.7**

Table S1. Total hydroxyl contents of SWKL (quantitative ^{31}P NMR).

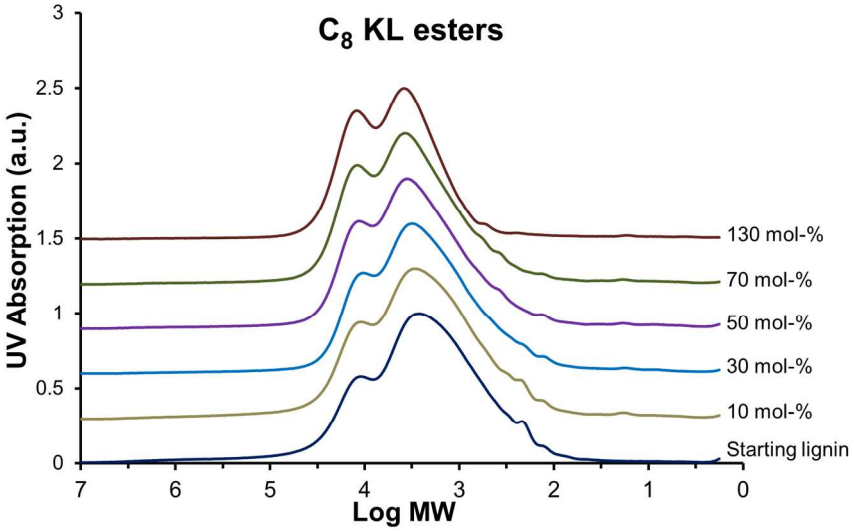

Figure S1. Molecular weight distributions of SWKL and 10-130 mol-% loaded C_8 KL esters. All GPC samples treated with acetobromination.

Sample	AcylCl loaded mol-%	M_n g/mol	M_w g/mol	PDI -
SWKL	-	2 100	19 000	8.9
C_2 KL esters	10	2 200	15 000	7.0
	30	2 100	10 000	4.9
	50	2 200	11 000	5.2
	70	2 300	16 000	6.9
	130	2 400	11 000	4.8
C_8 KL esters	10	2 200	13 000	5.8
	30	2 200	7 000	3.2
	49	2 400	11 000	4.4
	69	2 600	9 000	3.5
	130	3 000	7 000	2.3
C_{12} KL esters	10	2 100	11 000	5.5
	30	2 600	14 000	5.6
	49	2 800	11 000	4.0
	69	3 000	13 000	4.3
	130	4 100	11 000	2.6
C_{16} KL esters	10	2 400	12 000	5.0
	30	2 800	13 000	4.6
	49	3 000	10 000	3.4
	69	2 800	10 000	3.6

Table S2. GPC data of SWKL and C_2-C_{16} KL esters after acetobromination treatment. The 69 mol-% substituted C_{16} KL ester caused steep pressure buildup in the system and the data is unreliable, and the 130 mol-% substituted ester was not tested due to this issue. The problem on the GPC setup could have affected the M_w (and thus PDI) values of the other higher loaded KL esters too.

Sample	AcylCl loaded mol-%	Aliphatic OH esterified mol-%	Condensed phenolic OH esterified mol-%	Noncondensed phenolic OH esterified mol-%	Total phenolic OH esterified mol-%
C_2 KL esters	30	36	34	24	29
	50	55	47	39	43
	70	68	61	58	59
C_8 KL esters	30	34	29	17	23
	49	58	40	31	36
	69	73	57	52	55
C_{12} KL esters	30	34	28	19	23
	49	55	36	32	34
	69	73	53	54	54
C_{16} KL esters	30	31	28	18	23
	49	54	42	33	37
	69	73	58	57	57

Table S3. Hydroxyl group selectivity data of SWKL esterified with 30-70 mol-% C_2-C_{16} fatty acid chlorides (derived via quantitative ^{31}P NMR). 10 mol-% loaded samples were not considered for selectivity studies due to lower MW fraction of product washed away during purification.

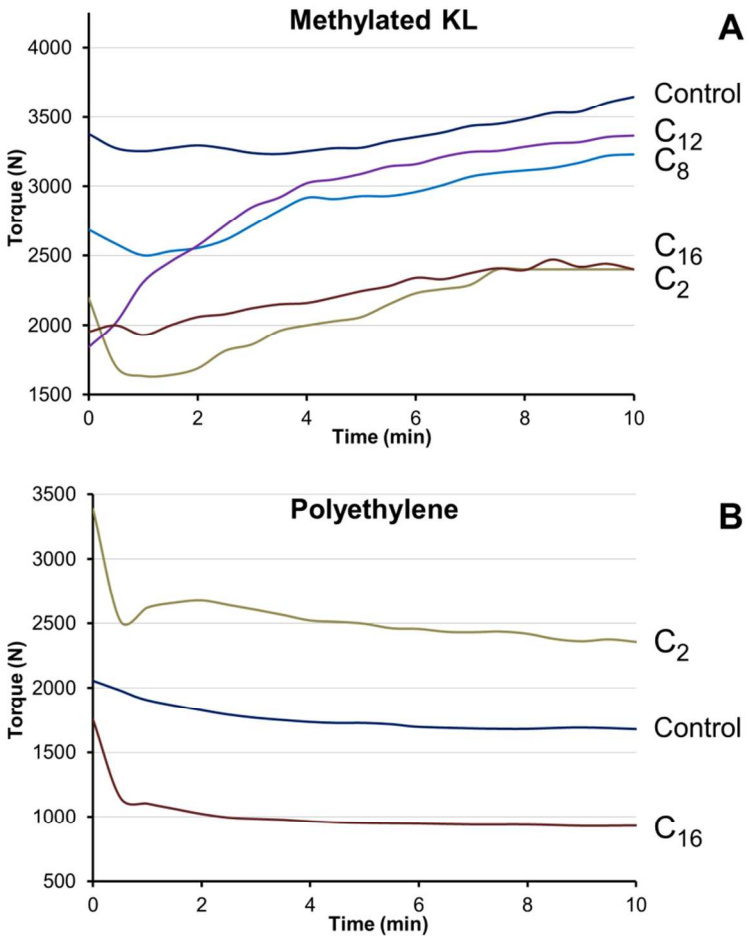

Figure S2. Extruder torque profiles for blends (sample:matrix 25:75 % w:w) of (A) methylated KL matrix with samples of methylated KL (control) and methylated C_2-C_{16} KL esters and (B) polyethylene matrix with samples of methylated KL (control) and methylated C_2 and C_{16} KL esters.