Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION FILE

Methylation of softwood and hardwood kraft lignins with chloromethane

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1 Molar mass distributions of methylated kraft lignin samples

Table S1. Average molar mass of methylated kraft lignin isolated during the optimization using chloromethane (0.5-g scale, 40 psi CH_3Cl).

Entry	Lignin	NaOH (mmol/g)	Temperature (°C)	Time (h)	H_2O (mL/g)	Average molar mass			
						M_w (SEC-MALS)	M_n (SEC-MALS)	M_w (SEC-RI)	M_n (SEC-RI)
-	SKL	-	-	-	-	15130	4440	7800	1670
-	HKL	-	-	-	-	8100	2210	4880	910
1	SKL	5	80	4	20	19660	7460	6640	1930
2	SKL	5	90	4	20	26100	7400	9350	2050
3	SKL	5	100	4	20	28580	8820	9460	2170
4	SKL	5	110	4	20	37650	9670	13310	2260
5	SKL	6	90	4	20	18870	6360	10080	1340
6	SKL	6	100	4	20	26800	6760	9640	2140
7	SKL	6	110	4	20	36550	8300	11590	2310
8	SKL	6	110	3	20	27600	7160	11170	2070
9	SKL	7	90	4	20	20730	7260	11480	1400
10	SKL	7	110	3	20	27300	7970	15100	1900
11	SKL	6	90	4	10	20000	7540	10800	1730
12	SKL	6	90	4	8	23200	7720	11400	1470
13	SKL	7	90	4	10	21200	7480	10870	1460
14[a]	SKL	7	90	4	9	21100	5500	8400	1490
15[a]	HKL	7	90	4	9	11300	3440	5280	720
16[b]	SKL	8	110	4	10	15100	4320	8330	1680

[a] 100-g scale. [b] Reaction done in the absence of CH_3Cl.

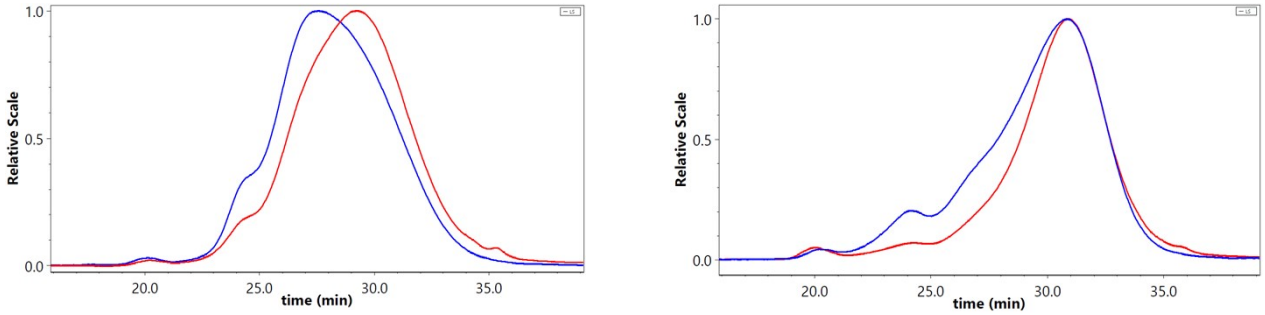

Figure S1. SEC-MALS profiles of A) SKL (red) and methylated SKL (blue) and of B) HKL (red) and methylated HKL (blue).

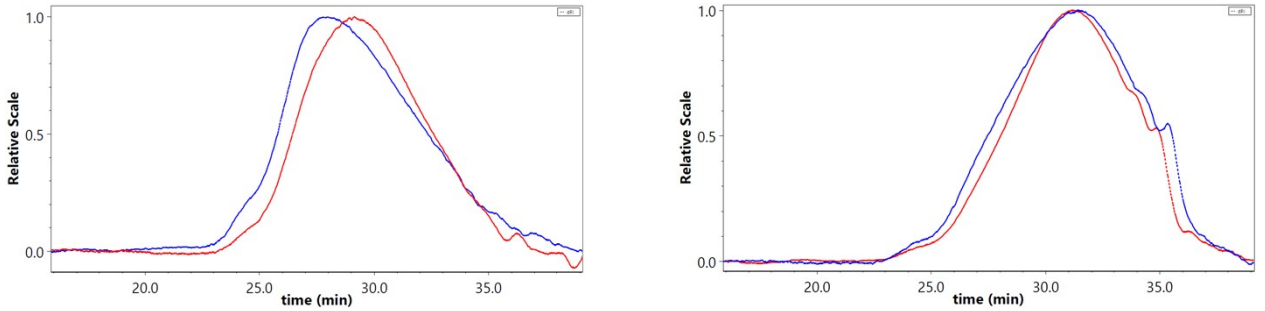

Figure S2. SEC-RI profiles of A) SKL (red) and methylated SKL (blue) and of B) HKL (red) and methylated HKL (blue).

2 DSC thermograms

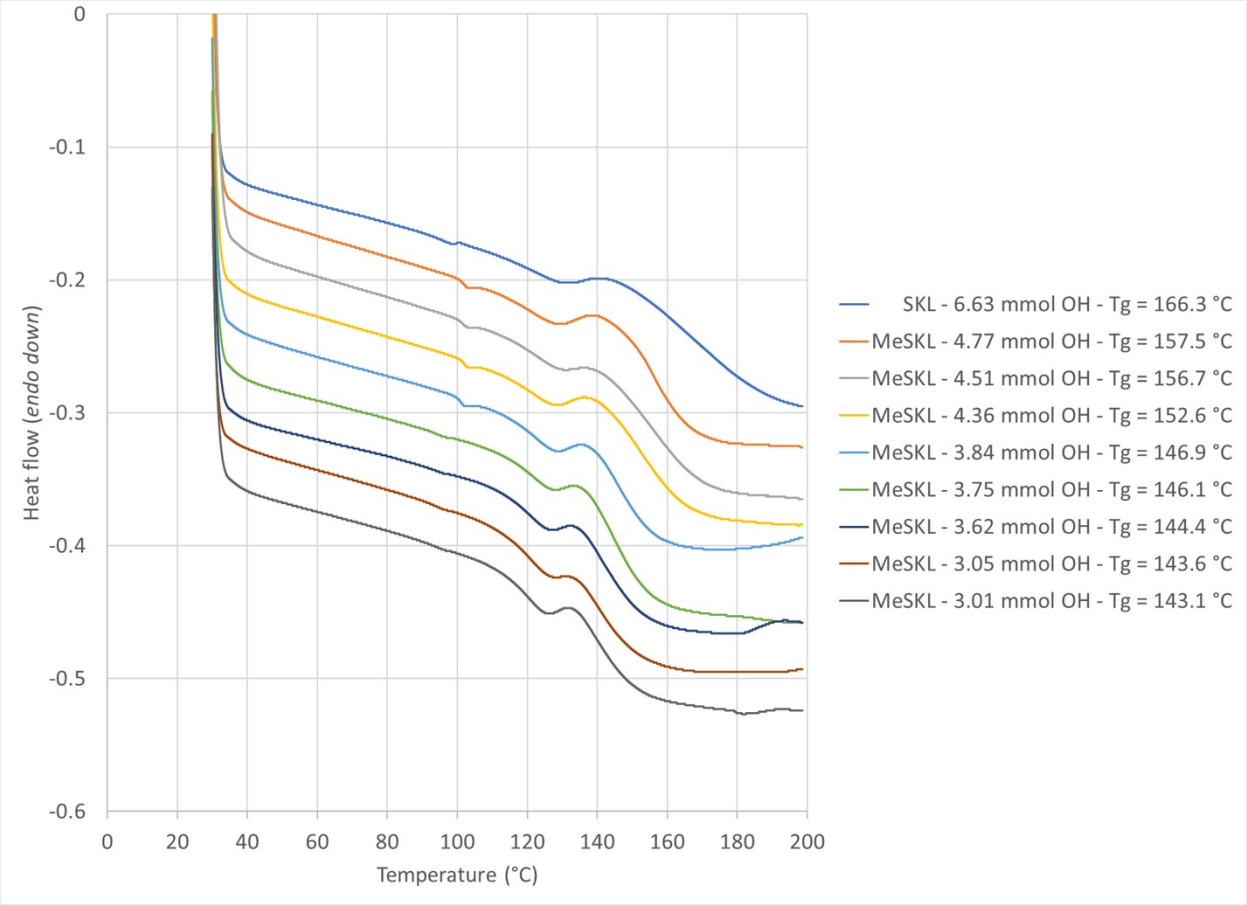

Figure S3. DSC thermograms of SKL and of various methylated SKL samples.

3 ^{31}P NMR spectra

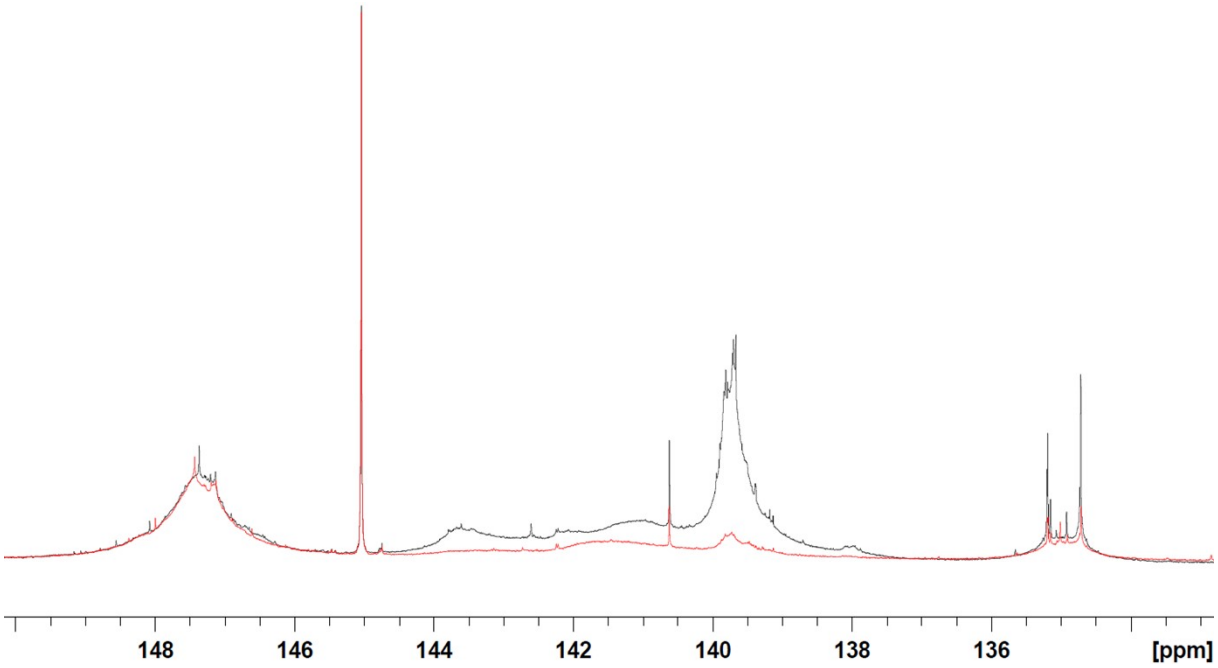

Figure S4. ^{31}P NMR spectra of SKL (black) and of methylated SKL (red).

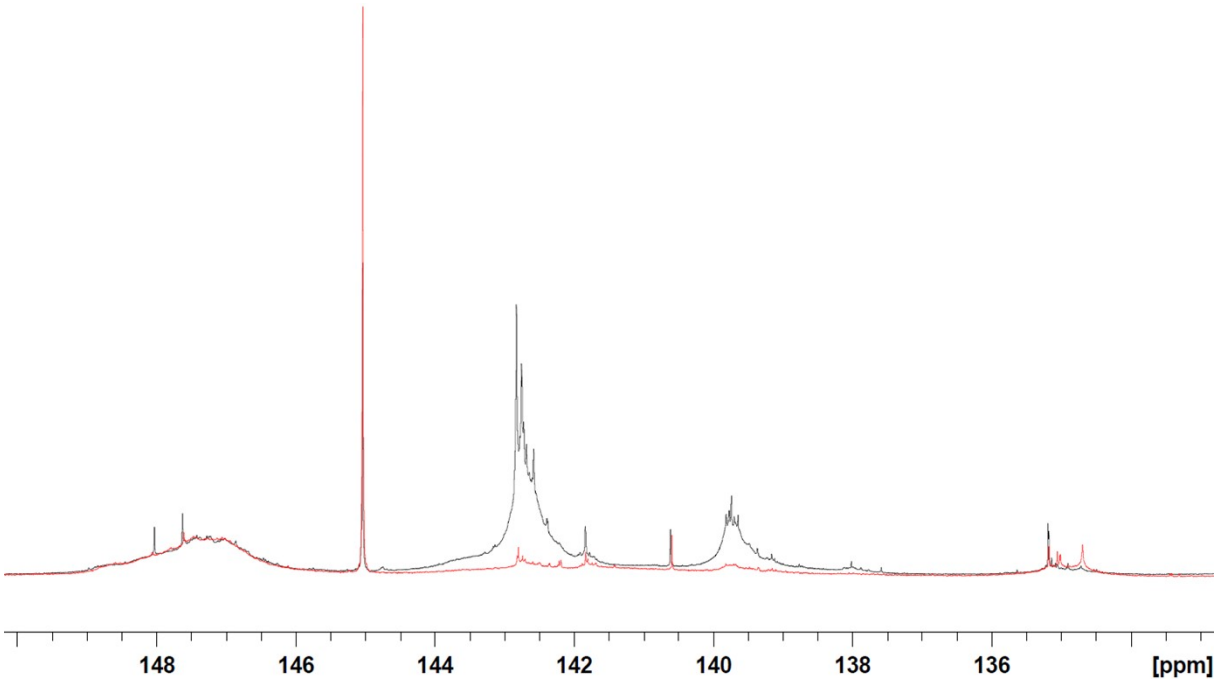

Figure S5. ^{31}P NMR spectra of HKL (black) and of methylated HKL (red).

4 ^{1}H NMR spectra

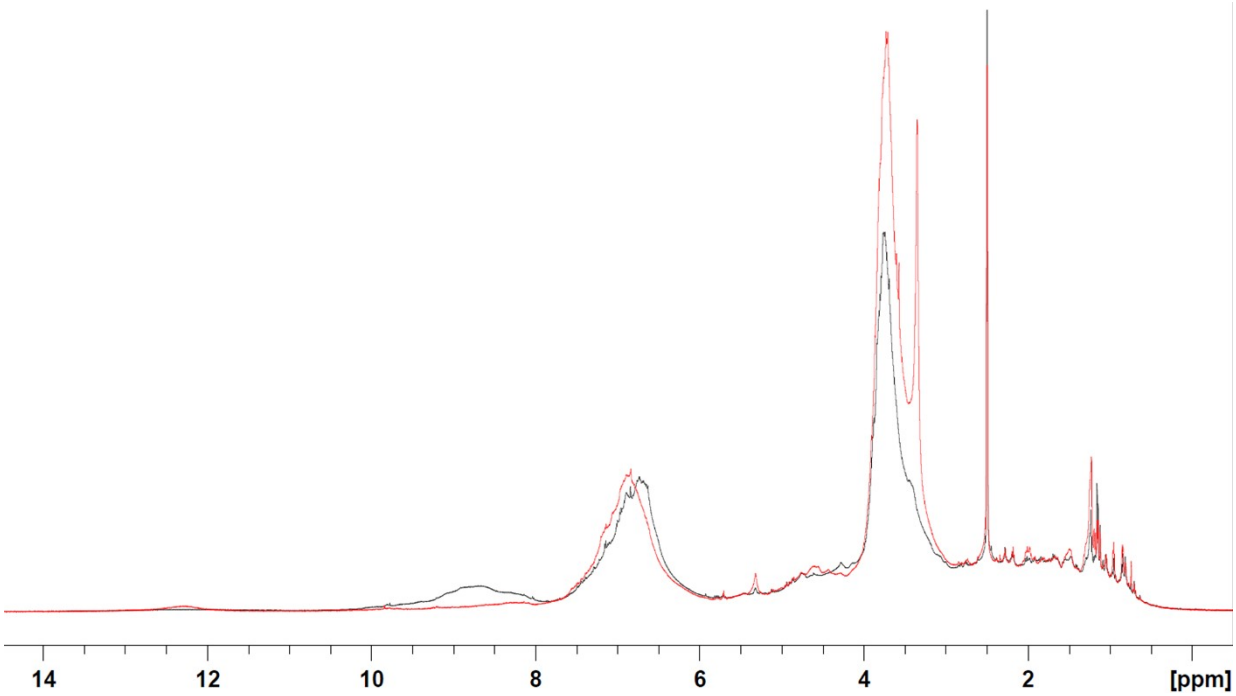

Figure S6. ^{1}H NMR spectra of SKL (black) and of methylated SKL (red).

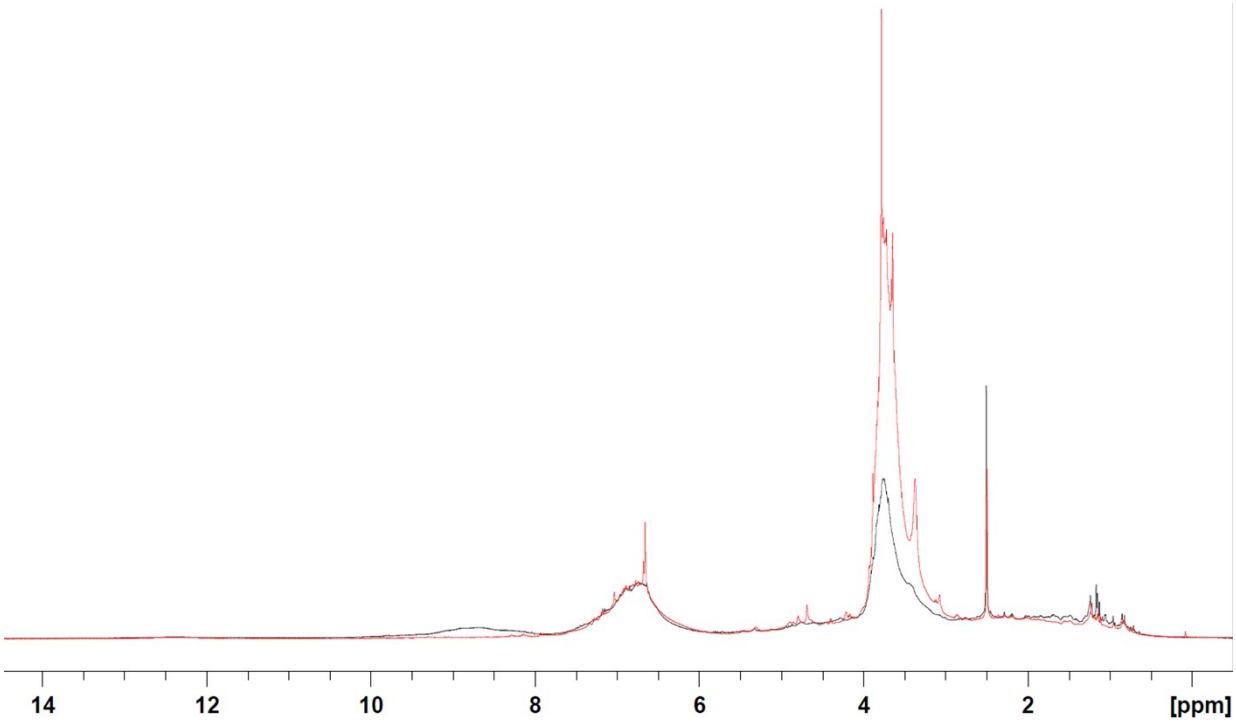

Figure S7. ^{1}H NMR spectra of HKL (black) and of methylated HKL (red).

5 ^{13}C NMR spectra

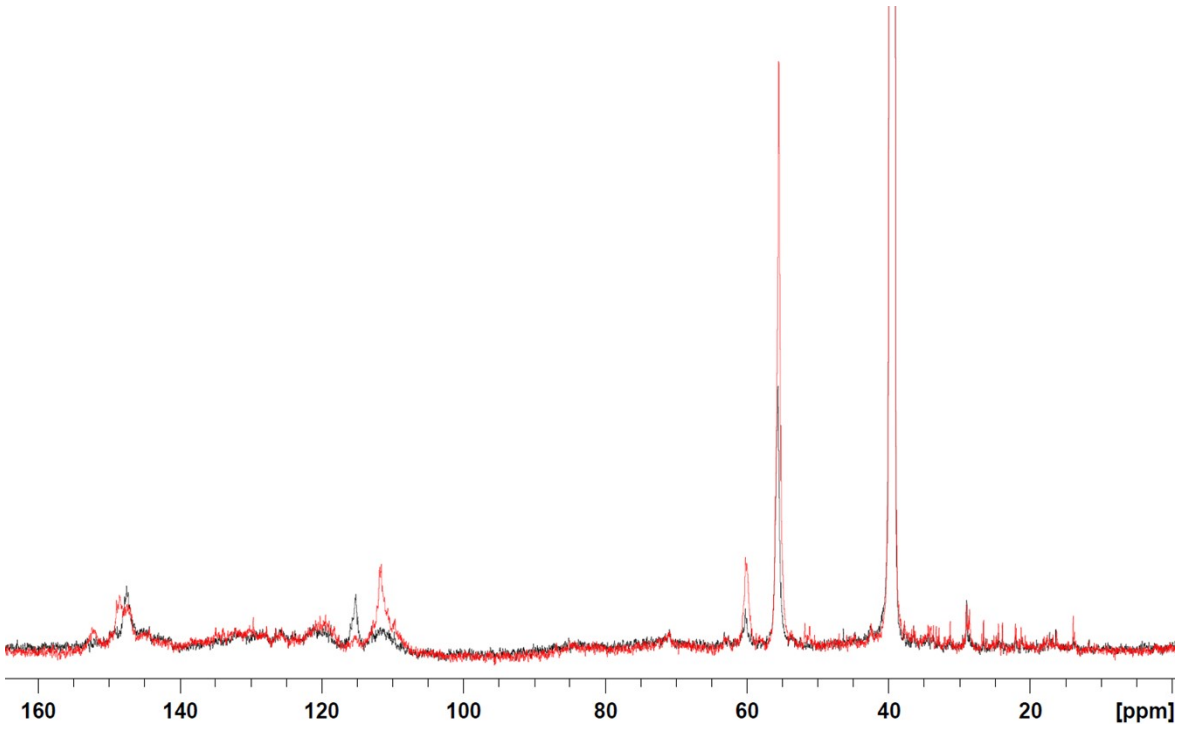

Figure S8. ^{13}C NMR spectra of SKL (black) and of methylated SKL (red).

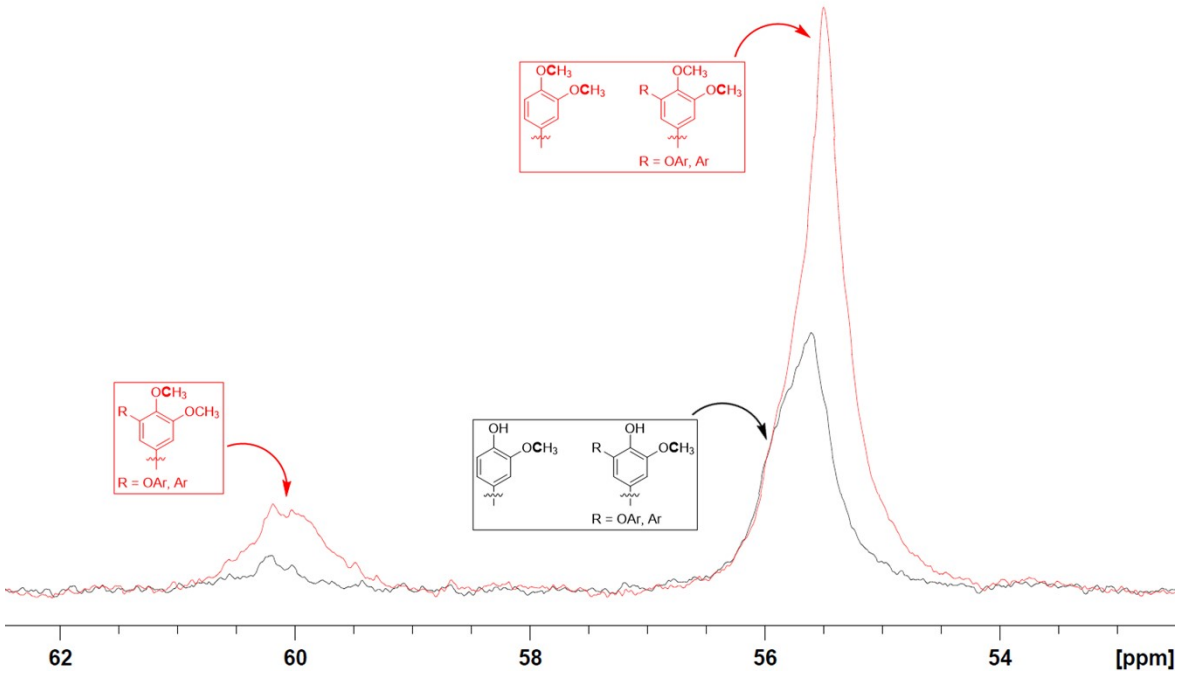

Figure S9. Zoomed fraction of the ^{13}C NMR spectra of SKL (black) and of methylated SKL (red) with carbon assignments.

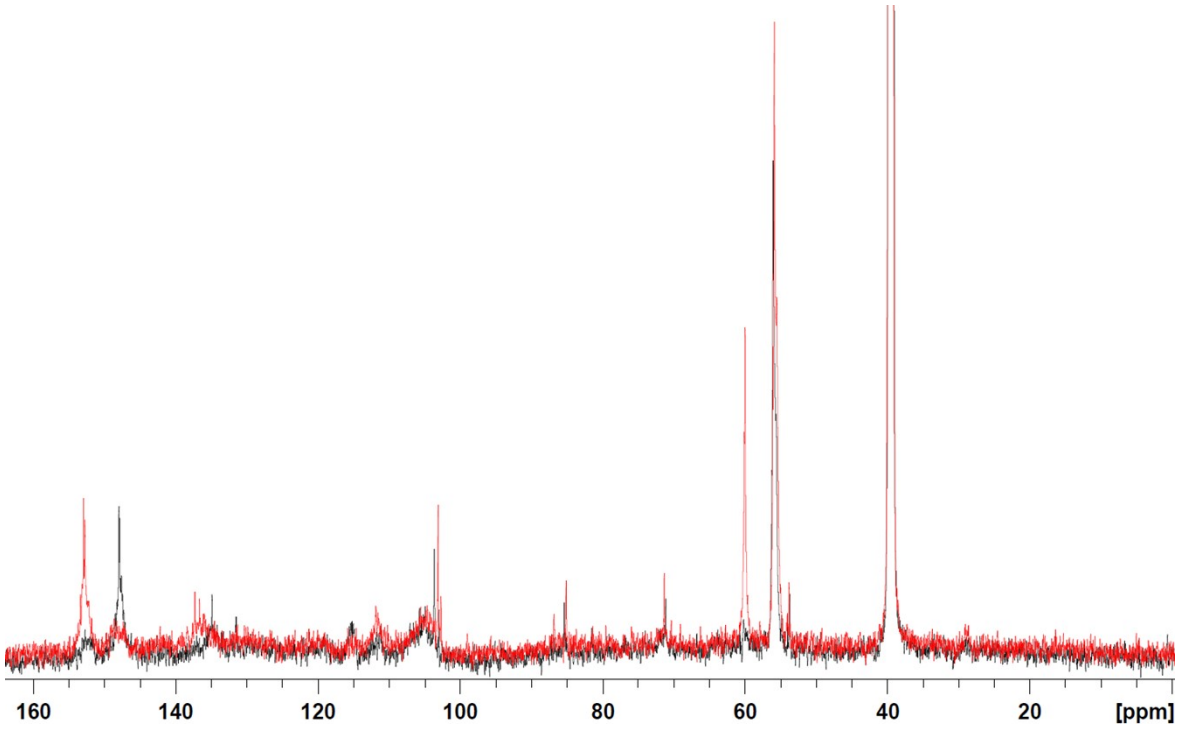

Figure S10. ^{13}C NMR spectra of HKL (black) and of methylated HKL (red).

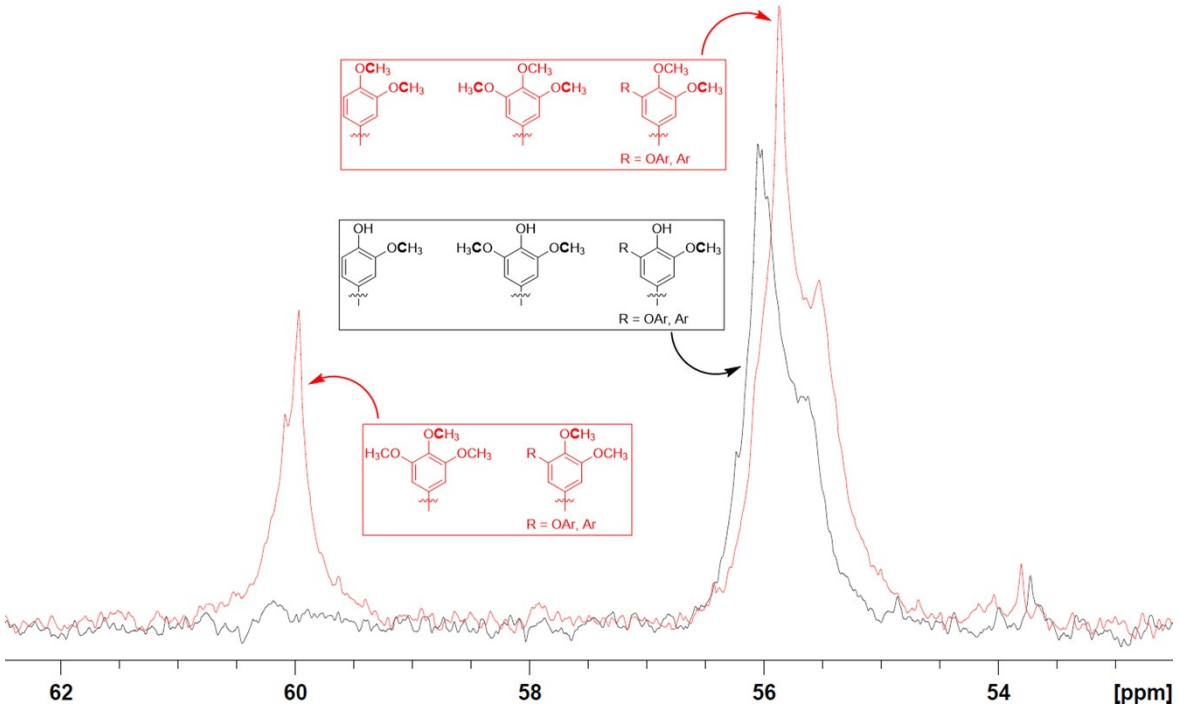

Figure S11. Zoomed fraction of the ^{13}C NMR spectra of HKL (black) and of methylated HKL (red) with carbon assignments.

6 HSQC NMR spectra

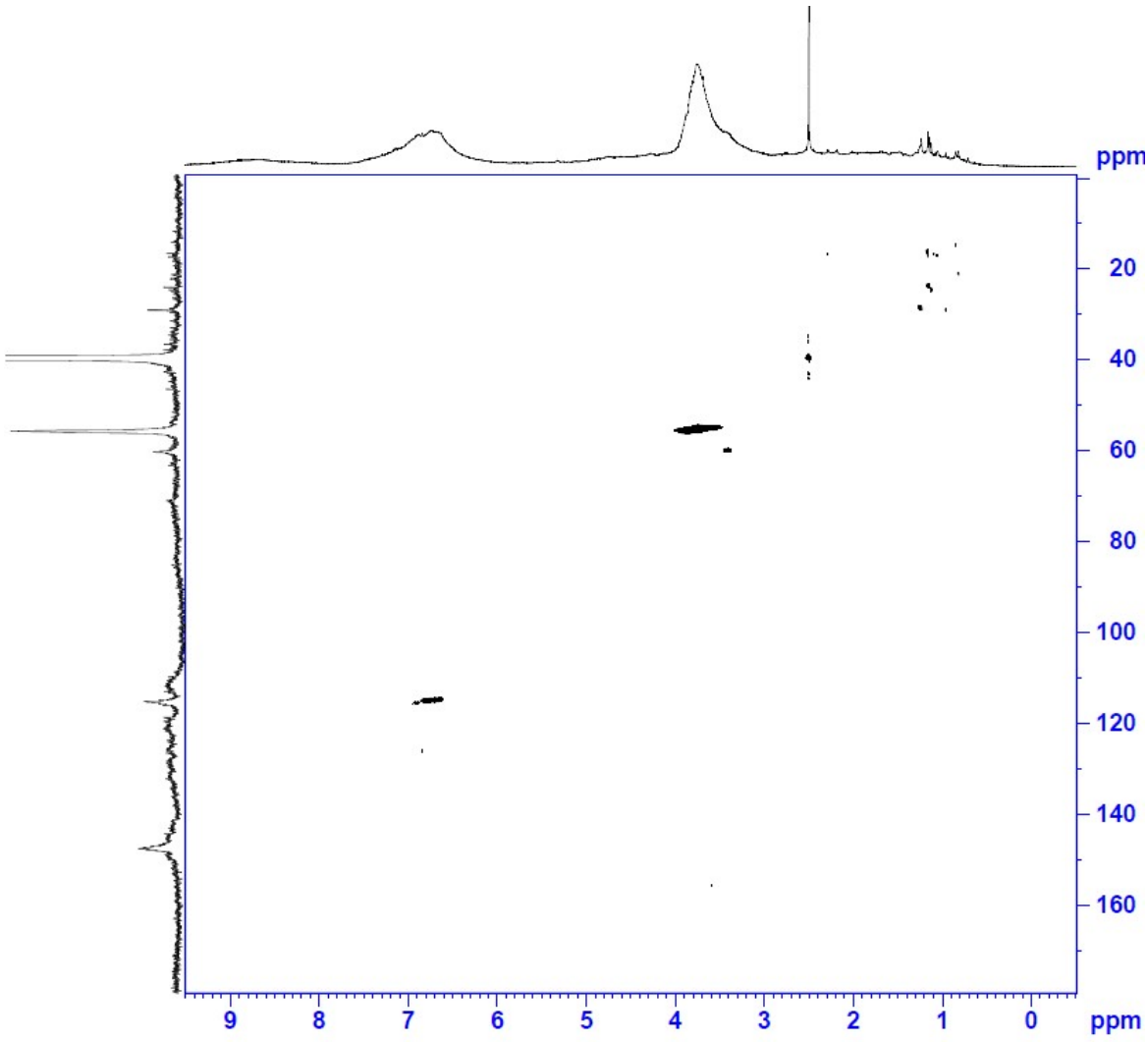

Figure S12. HSQC NMR spectra of SKL.

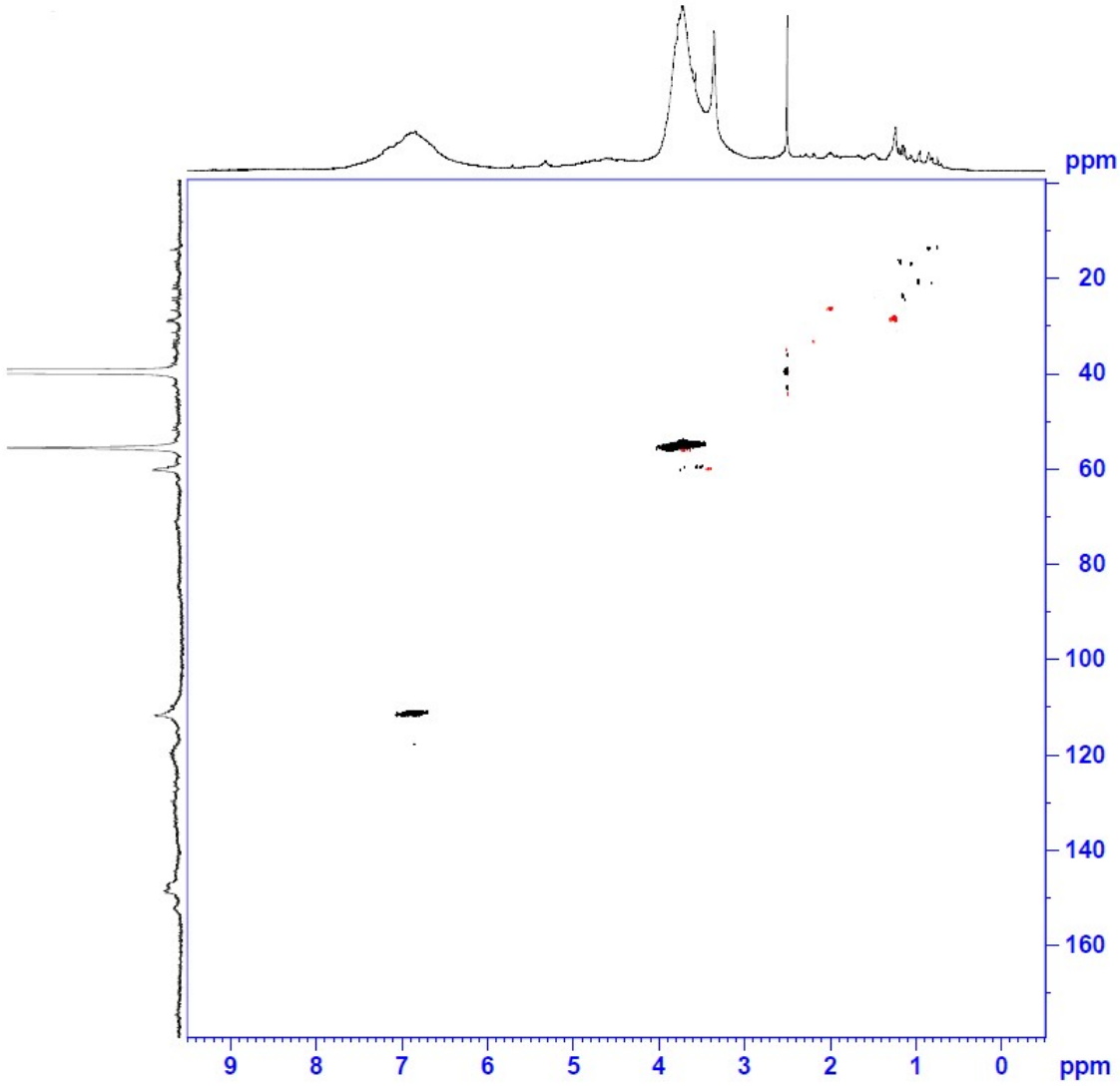

Figure S13. HSQC NMR spectra of methylated SKL.

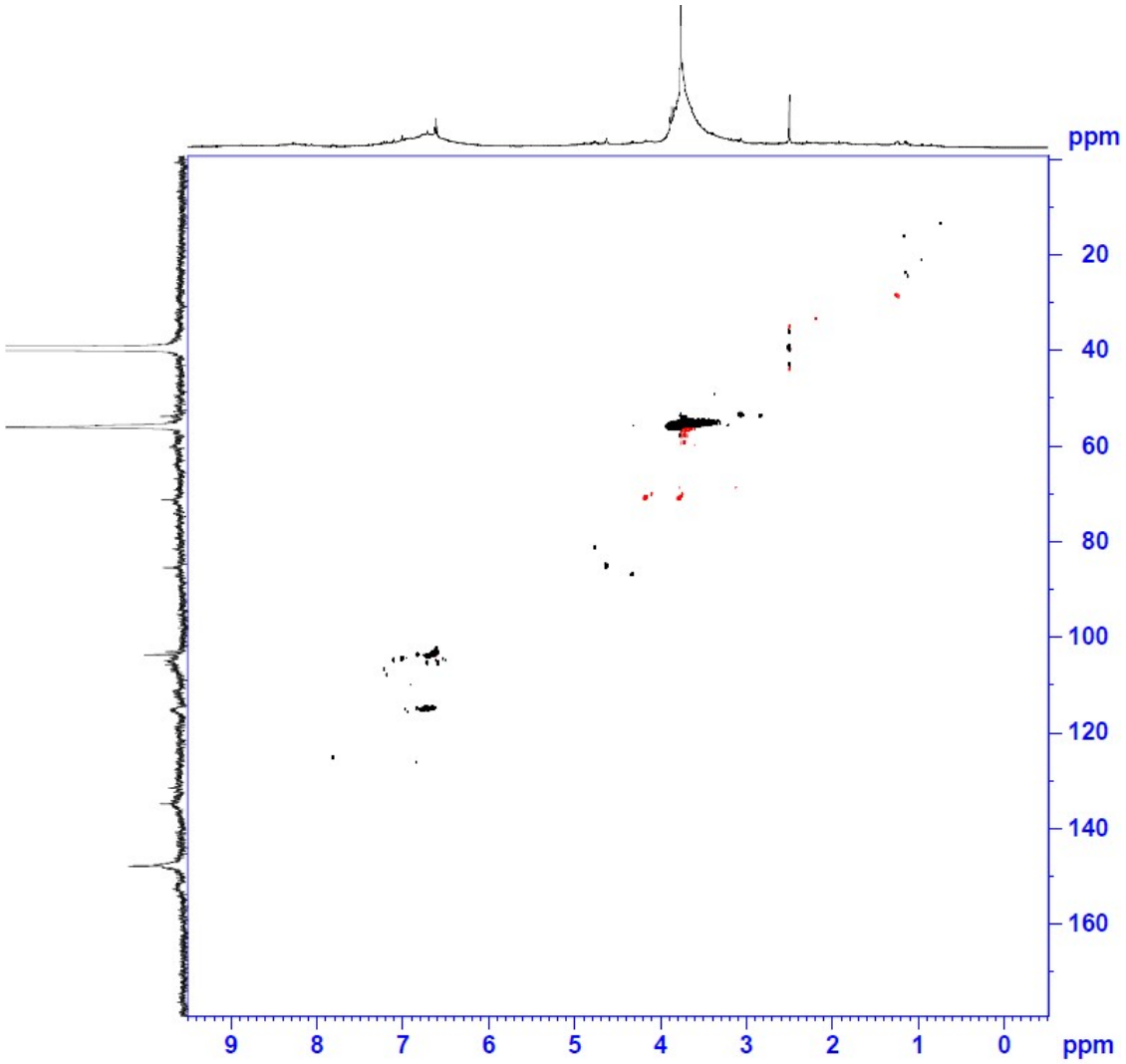

Figure S14. HSQC NMR spectra of HKL.

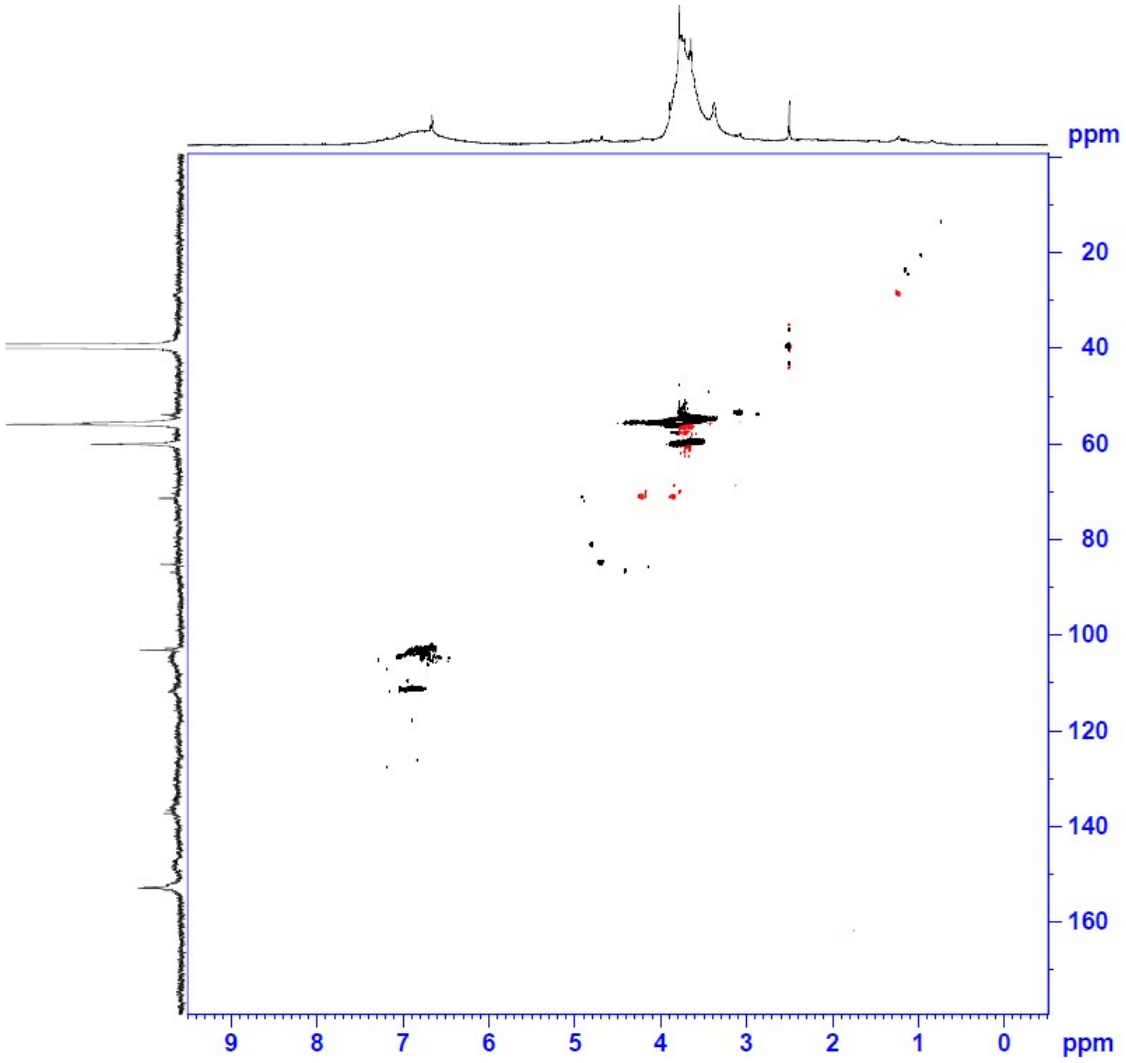

Figure S15. HSQC NMR spectra of methylated HKL.

7 FTIR spectra

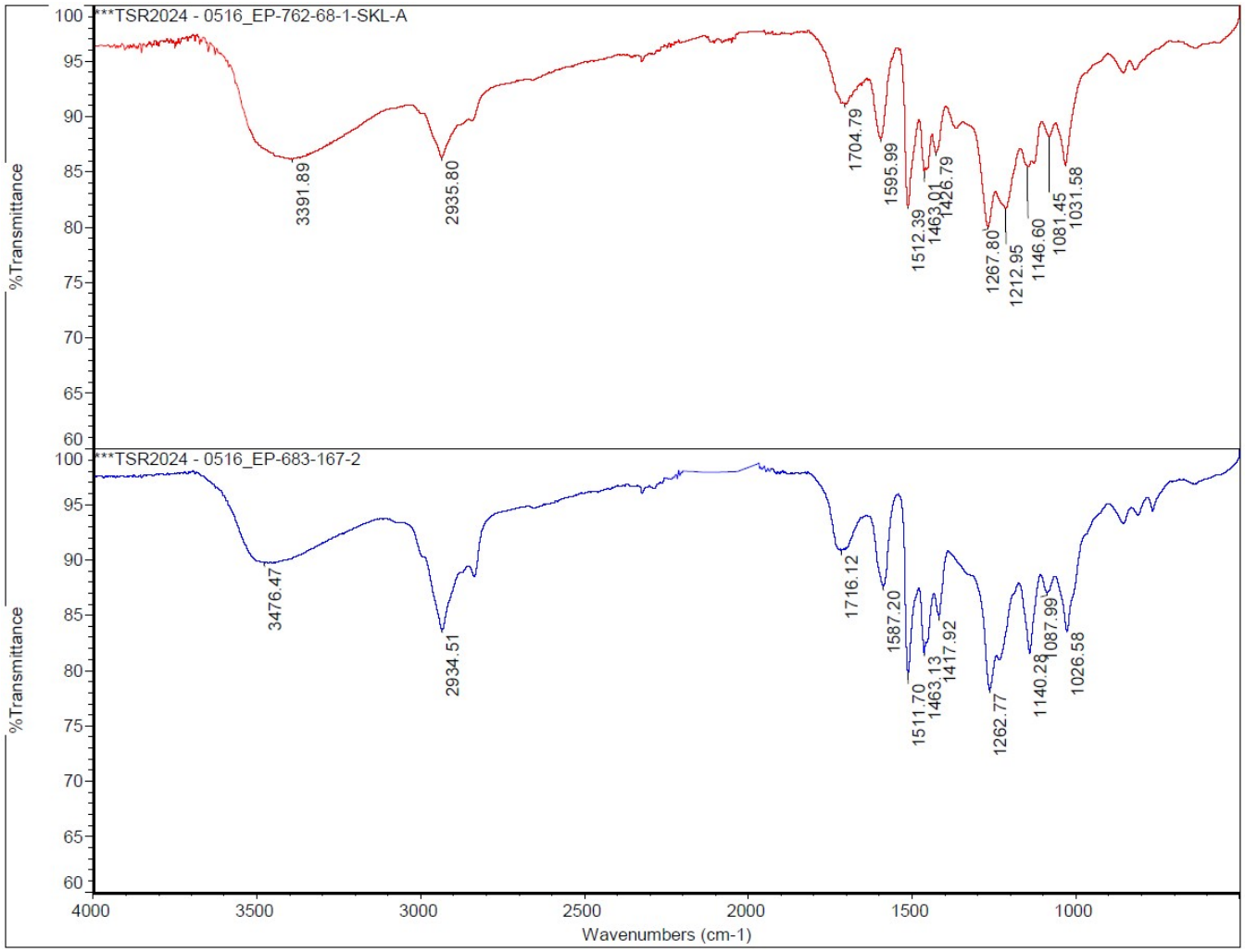

Figure S16. FTIR spectra of SKL (red) and of methylated SKL (blue).

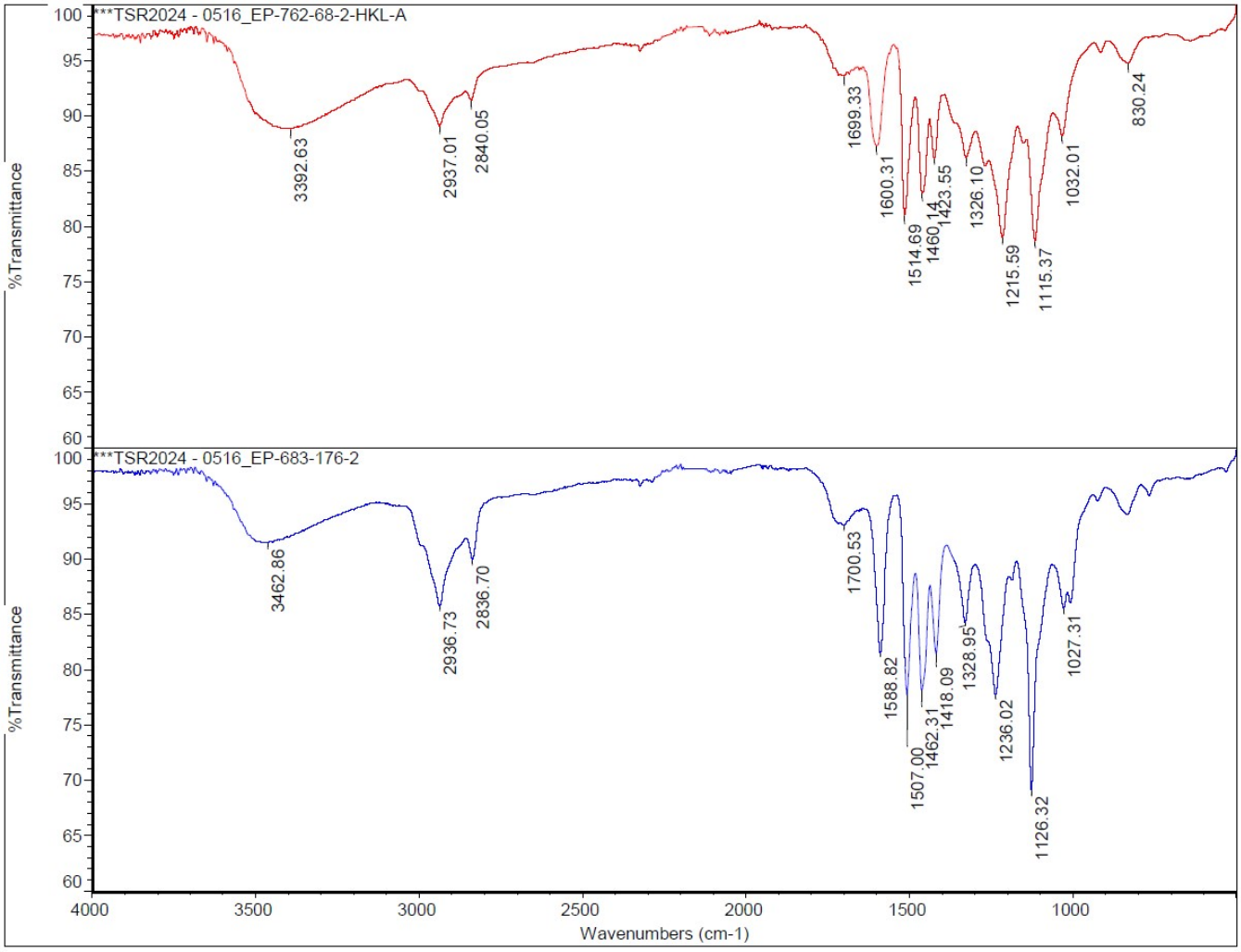

Figure S17. FTIR spectra of HKL (red) and of methylated HKL (blue).