Electronic Supporting Information

Thermal and mechanical properties of esterified lignin in various polymer blends

Alexander Orebom[a], Davide Di Francesco[b], Patrick Shakari[c], Joseph Samec[a,b] and Clara Pierrou*[,a]

[a] RenFuel K2B Materials AB, Rapsgatan 25, 75450 Uppsala (Sweden)

[b] Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Svante Arrhenius väg 16C, 106 91 Stockholm (Sweden)

[c] Department of Polymer Chemistry, Ångström laboratory, Uppsala University, Lägerhyddsvägen 1, 751 21 Uppsala (Sweden)

Thermogravimetric analysis

Thermogravimetric analysis (TGA) was performed on a Mettler TGA/DSC1 system using a temperature programme from 50°C to 600°C (heating rate: 10°C min^{-1}) in nitrogen atmosphere (flow rate: 80 mL min^{-1}). The samples were held at constant temperature in 5 min, followed by an air flow of 80 mL min-1 at 600°C for 10 minutes. Sample size 5 mg.

^exo

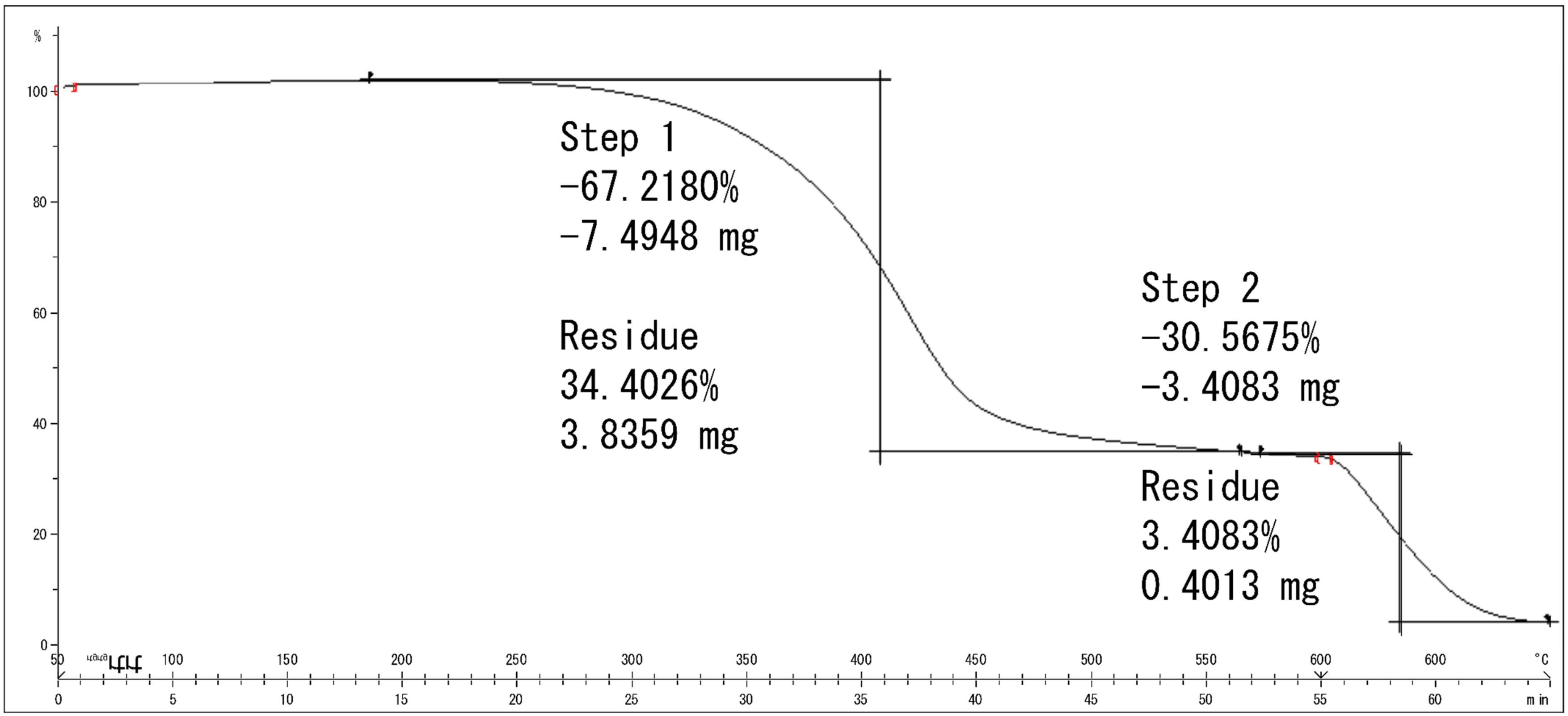

Figure S1 TGA curve for pure lignin ester.

Differential scanning calorimetry

Differential scanning calorimetry (DSC) for the blends was performed on a DSC Q2000 system using a heat/cool/heat programme from -25°C to 200°C (heating rate: 10°C min -1, cooling rate: 5°C min -1). DSC for pure lignin ester was performed on a Mettler DSC1 system using a heating programme from 25°C to 175°C (heating rate: 10°C min -1) in nitrogen atmosphere (flow rate: 80 mL min $^{-1}$). Sample size 5 mg.

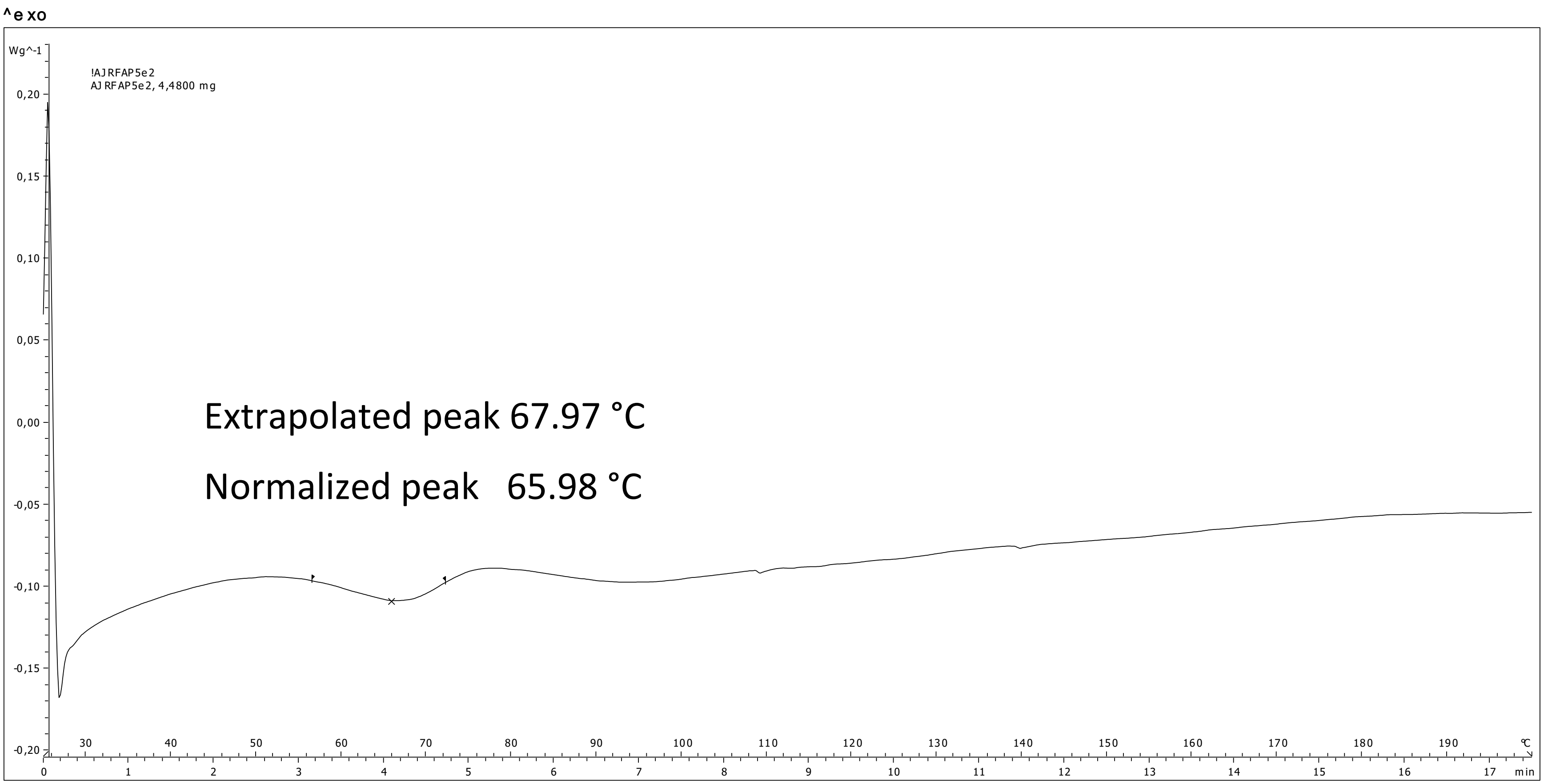

Figure S2 DSC curve for pure lignin ester.

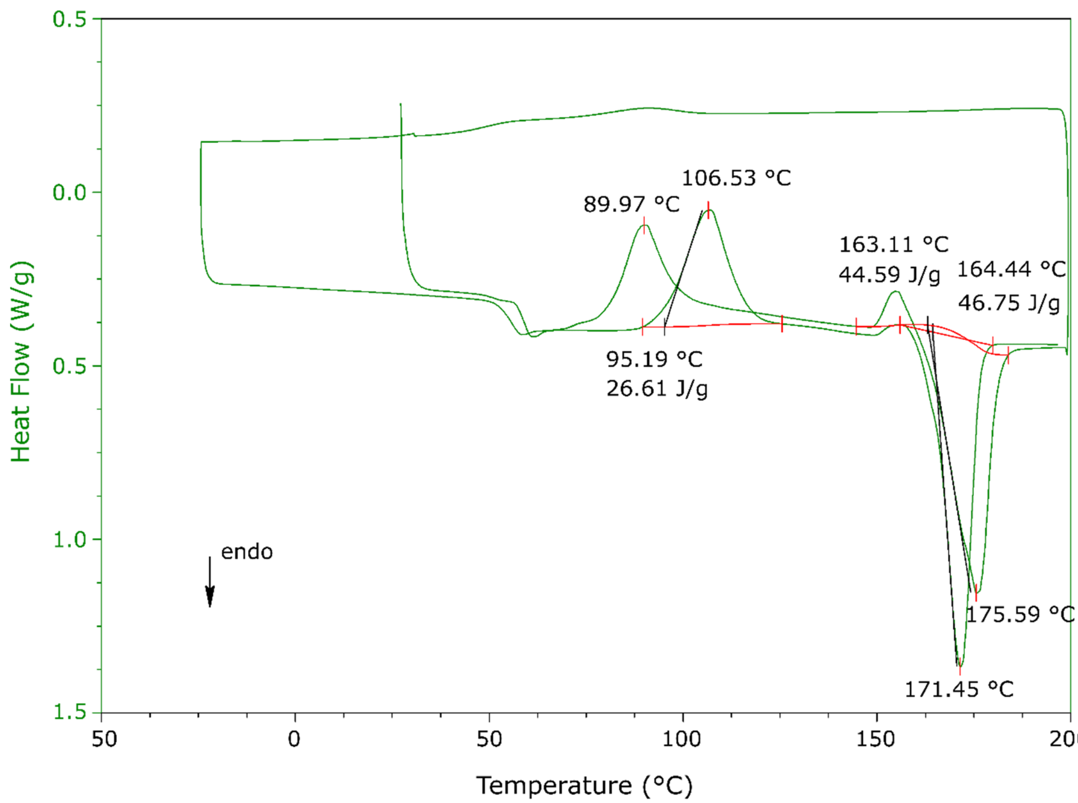

Figure S3 DSC curve for PLA – lignin ester using heat/cool/heat programme from -25°C to 200°C (heating rate: 10°C min^{-1}, cooling rate: 5°C min^{-1}).

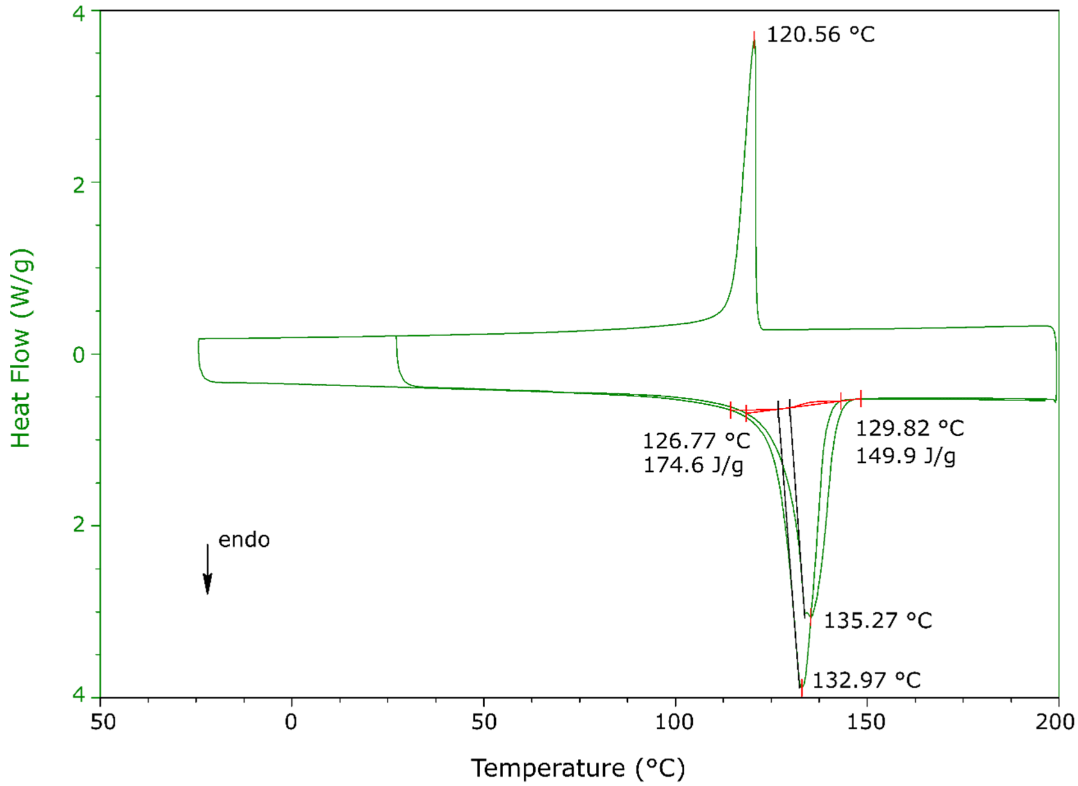

Figure S4 DSC curve for HDPE – lignin ester using heat/cool/heat programme from -25°C to 200°C (heating rate: 10°C min^{-1}, cooling rate: 5°C min^{-1})

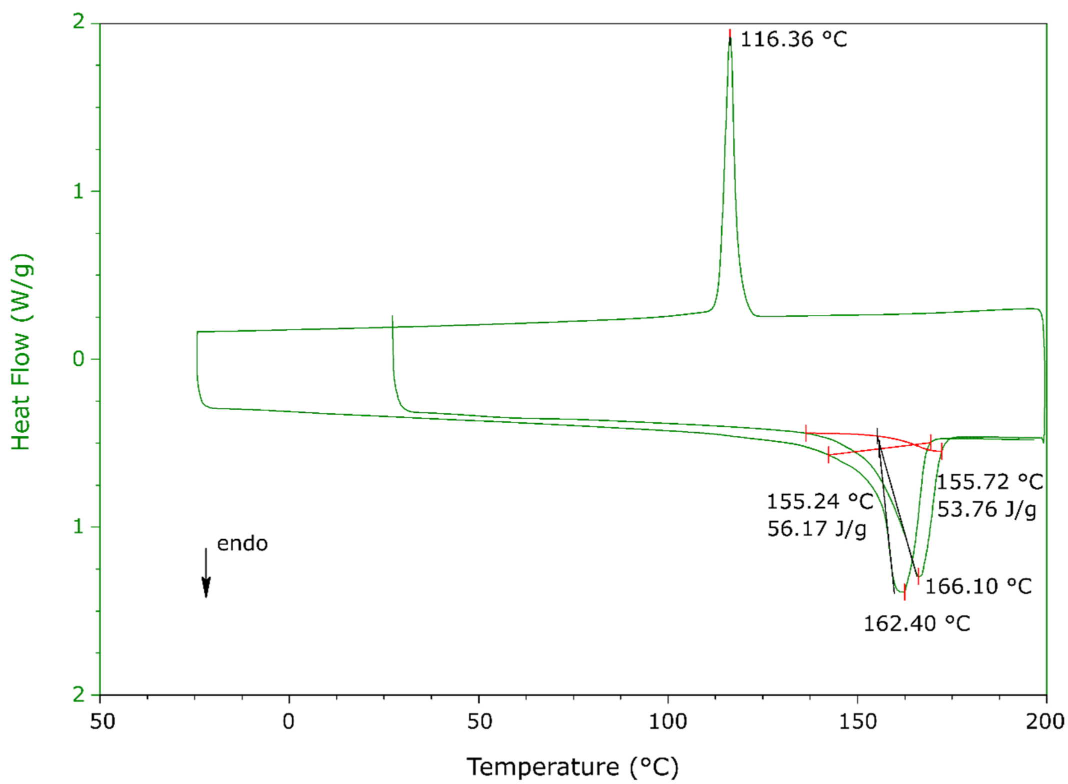

Figure S5 DSC curve for PP – lignin ester using heat/cool/heat programme from -25°C to 200°C (heating rate: 10°C min^{-1}, cooling rate: 5°C min^{-1}).

FT-IR

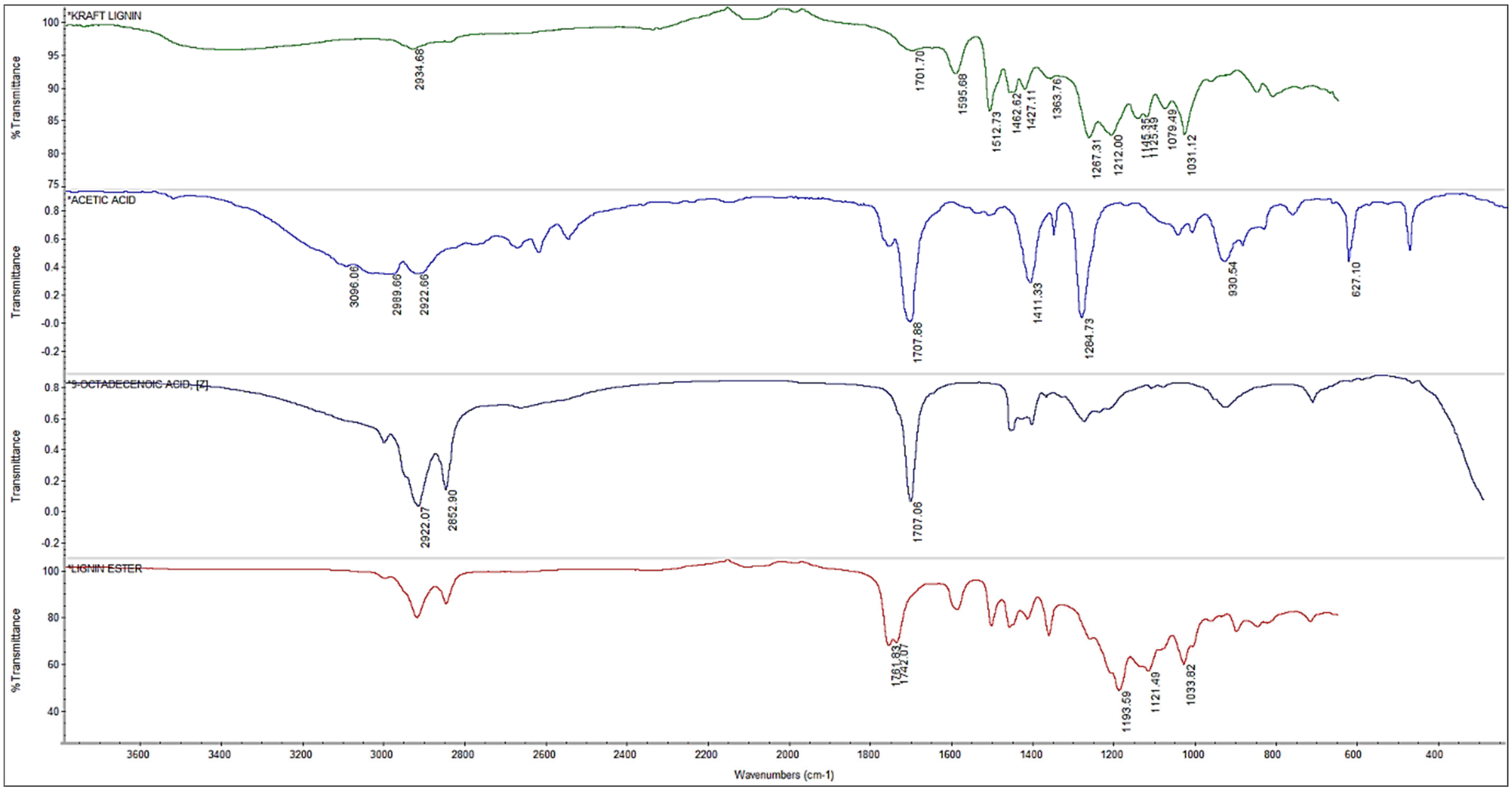

Figure S6 FT-IR spectra of (from top to bottom) kraft lignin, acetic acid, oleic acid, and lignin ester.

NMR

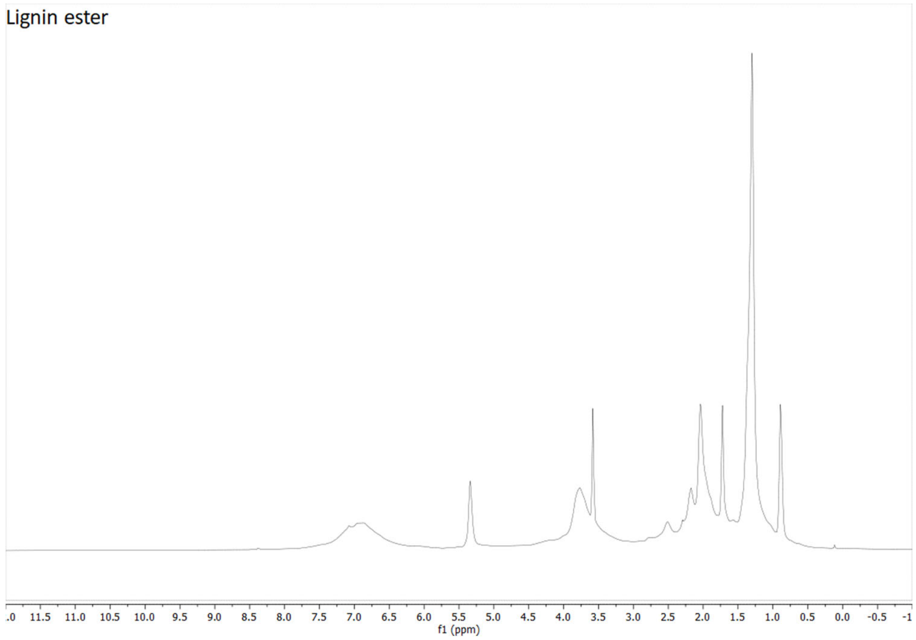

Figure S7 ^{1}H NMR spectrum of lignin ester in d8-THF.

Figure S 8 HMBC spectrum of lignin ester in d8-THF.

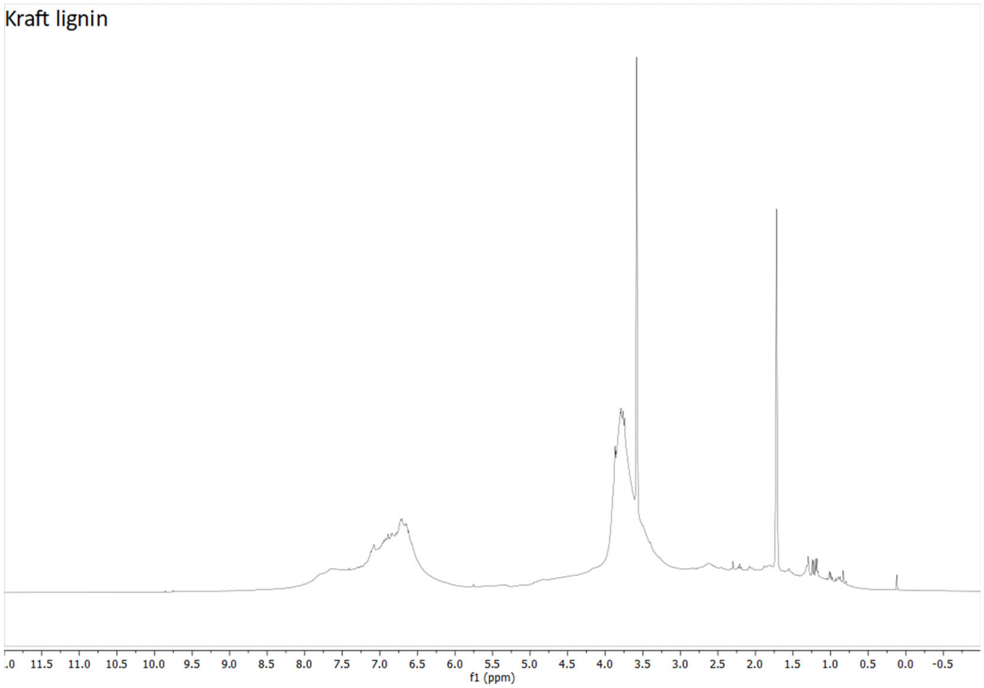

Figure S9 ^{1}H NMR spectrum of Kraft lignin in d8-THF.

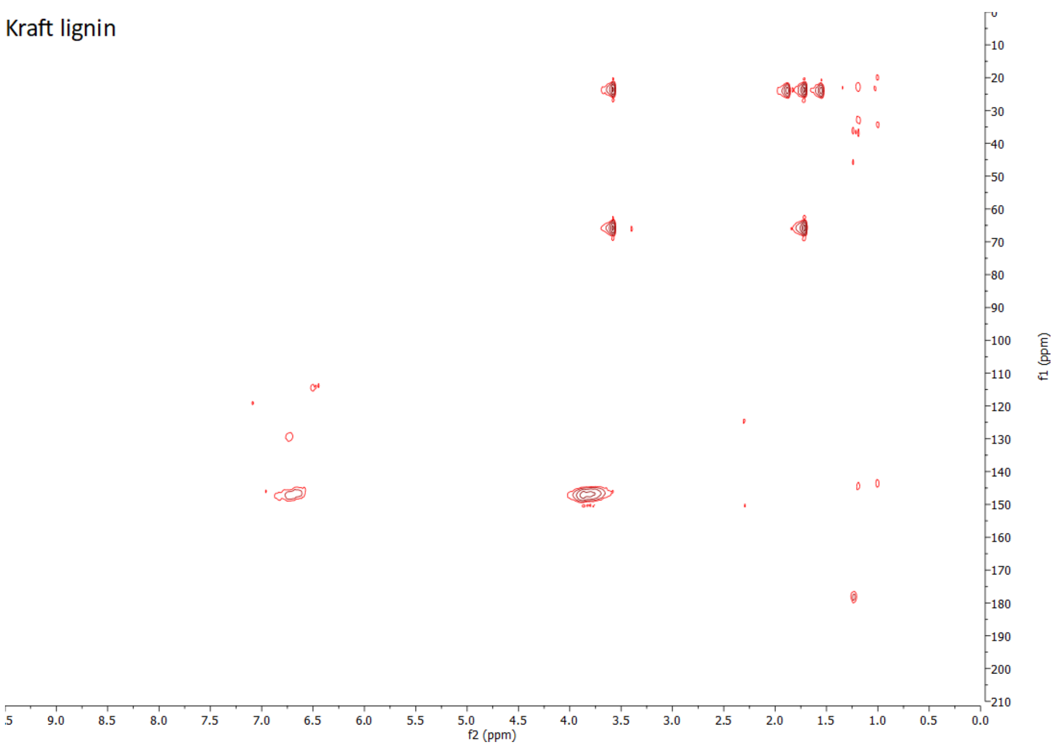

Figure S10 HMBC spectrum of Kraft lignin in d8-THF.

GPC

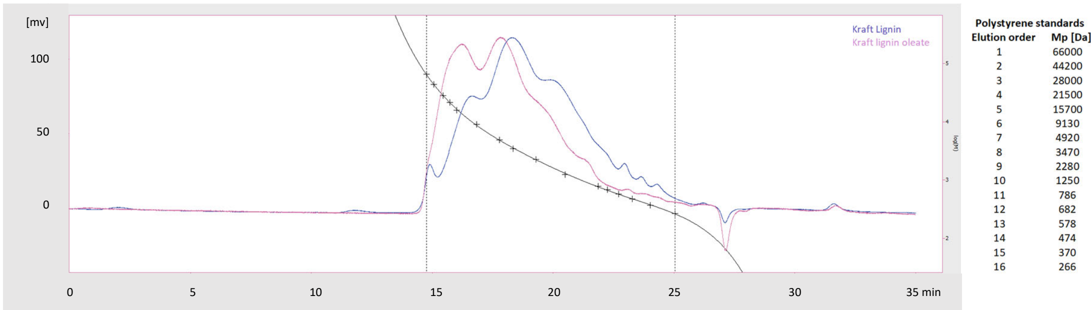

Figure S11 GPC chromatogram of lignin ester (pink) and kraft lignin (blue).

Mechanical properties

Polymer blends of lignin esters in PP, HDPE and PLA were prepared using a Coperion twin screw compounder to mix blends with a 20% lignin ester to plastic proportion and pure samples of PP, HDPE and PLA as a reference material at 180°C. The obtained extrudates were cut using a granulator into pieces followed by injection moulding of the pellets into dumbbell shaped samples using an Engel injection moulder at 185°C with reference to ISO 527-2 specifications. The dumbbell samples were used to determine the tensile properties of each lignin ester sample compared to the reference, respectively. Tensile tests were performed using a MTS20/M system according to ISO 527-2 (1 mm min^{-1} /50 mm min^{-1}), and impact strength tests were performed using an Instron CEAST 9050 instrument according to ISO 179 type A using a 0.5 J hammer with sample sizes of 3.94x8x8 mm.

Table S1 Numerical values for mechanical properties of the various blends.

			HDPE – LE		PP – LE		PLA – LE	
Tensile properties	Method	Unit	Value	δ	Value	δ	Value	δ
Young's modulus	ISO 527-2	MPa	1260	18	1637	35	3248	31
Stress at yield	ISO 527-2	MPa	26.3	0.2	29.4	0.2	59.4	0.2
Strain at yield	ISO 527-2	%	6.3	0.2	3.9	0.1	2.1	0.1
Impact resistance (+23 °C)								
Charpy. notched.	ISO 179	kJ/m^2	2.7	0.7	2.8	0.5	2.1	0.6
Charpy. unnotched.	ISO 179	kJ/m^2	25.6	2.8	17.5	1.1	14.8	1.6

Value intended as mean value and δ as standard deviation.

Table S2 Numerical values for mechanical properties of the reference polymers.

Tensile properties	Unit	**HDPE**	**PP**	**PLA**
Young's modulus	MPa	1200	1500	3500
Stress at yield	MPa	27	34	60[1]
Strain at yield	%	8	9	2.4[1]
Impact resistance (+23 °C)				

Charpy. notched.	kJ/m^2	7	3	5

References

1 G. W. de Kort. L. H. C. Bouvrie. S. Rastogi and C. H. R. M. Wilsens. *ACS Sustain. Chem. Eng.*. 2020. **8**. 624–631.

2 Acetic acid. https://webbook.nist.gov/cgi/cbook.cgi?ID=C64197&Type=IR-SPEC&Index=2#IR-SPEC. (accessed 2 November 2020).

3 Oleic Acid. https://webbook.nist.gov/cgi/cbook.cgi?ID=C112801&Units=SI. (accessed 2 November 2020).