Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Carbon Fibre From Renewable Resources: The Role of Lignin Molecular Structure on its Blendability with Biobased Poly(Ethylene Terephthalate)

Anne Beaucamp[a], Yan Wang[a,b], Mario Culebras[a] and Maurice N. Collins*[a]

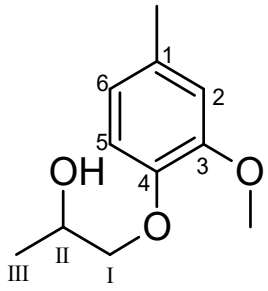

Figure S1: Chemical structure of a modified lignin unit

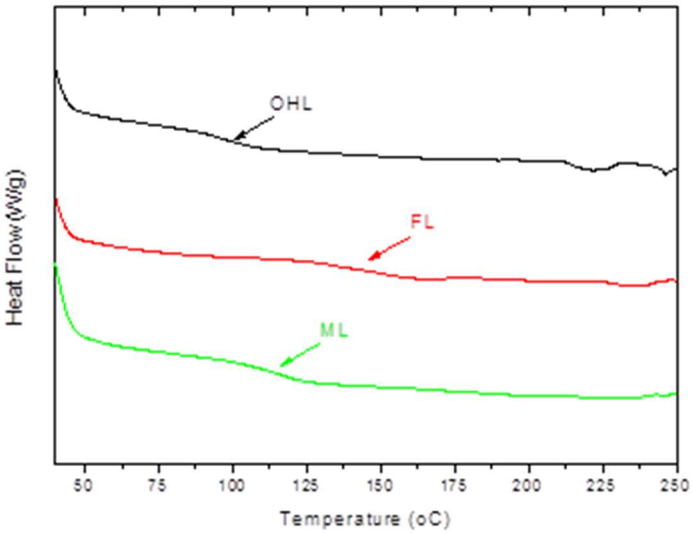

Figure S2: Glass transition temperature for OHL*, FL and ML* (Results from a previous study [33])

Table S1: Molecular Weights (Mn and Mw) and PolyDispersity Index (PDI) of the lignins examined in this work as determined by GPC and DSC analysis.

	M_n ($g.mol^{-1}$)	M_w ($g.mol^{-1}$)	PDI	Tg (°C)
OHL	842	3952	4.69	100
FL	925	6083	6.57	150
ML	2478	11357	4.58	110

Table S2: Assignment of the FTIR resonance bands as according to Faix [34]

Band (cm^{-1})	Chemical group
3390-3460	O-H stretching in Aromatic and Aliphatic groups
3000-2840	C-H stretching of methoxy groups, methyl and methylene groups in side chains
1696	C=O stretching of conjugated aldehydes and carboxylic acids
1599, 1514, 1424	Aromatic skeletal vibrations
1457	Aromatic methyl group vibrations
1370	Phenolic O-H Vibration
1326	Stretching at the ring, S > G
1212	C-O stretching in ether linkage
1152, 1112	Aromatic C-H in plane deformation
1030	Aliphatic O-H
912, 826	Aromatic C-H out of plane

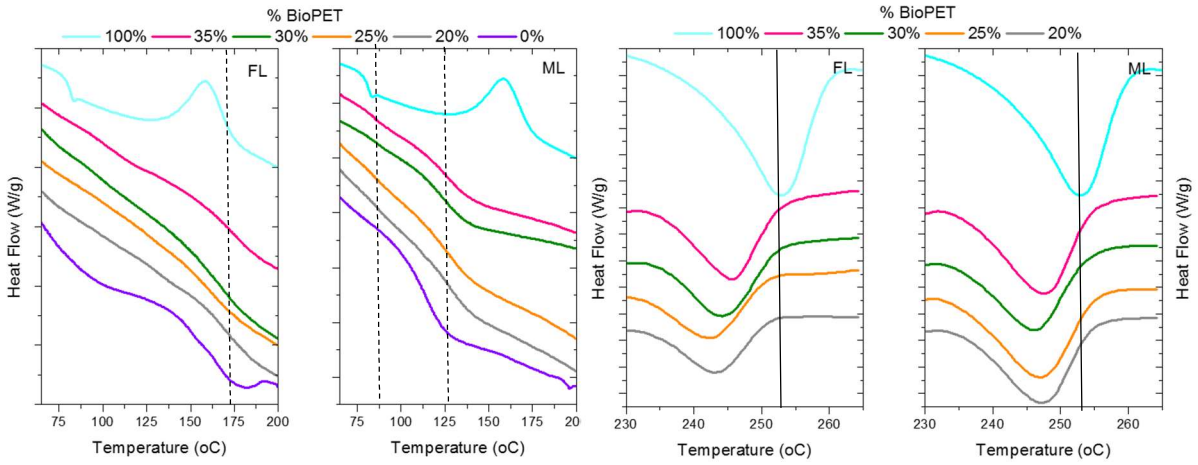

Figure S3: Evolution of the heat flow with temperature for FL and ML blends with BPET at various composition for the BPET melting transition.

TableS3: Calculation of the Group Molar Attraction Constant $\sum n_i F_i$ for OHL, ML and BPET repeat units

	F_i * ($(J.m^3)^{1/2}$. mol^{-1})	OHL		FL		ML		BPET	
		Number of groups n_i	$\sum n_i F_i$ ($(J.m^3)^{1/2}$. mol^{-1})	Number of groups n_i	$\sum n_i F_i$ ($(J.m^3)^{1/2}$. mol^{-1})	Number of groups n_i	$\sum n_i F_i$ ($(J.m^3)^{1/2}$. mol^{-1})	Number of groups n_i	$\sum n_i F_i$ ($(J.m^3)^{1/2}$. mol^{-1})
$-CH_3$	0.3032	0	0	0	0	2	0.6064	0	0
$-CH_2-$	0.2689	2	0.5378	3	0.8067	6	1.6134	2	0.5378
>CH-	0.1758	4	0.7032	6	1.0548	4	0.7032	0	0
=CH-	0.2485	0	0	0	0	0	0	0	0
$-O-CH_3$	0.236	3	0.708	4	0.944	3	0.708	0	0
-COO-	0.6677	0	0	0	0	0	0	2	1.3354
-O-	0.2351	2	0.4702	3	0.7053	4	0.9404	0	0
Aromatic CH	0.2395	5	1.1975	7	1.6765	5	1.1975	4	0.958
Aromatic C	0.2006	7	1.4042	11	2.2066	7	1.4042	2	0.4012
Aromatic Meta	0.0135	3	0.0405	5	0.0675	3	0.0405	0	0
Aromatic Para	0.0825	2	0.165	3	0.2475	2	0.165	1	0.0825
6-Membered Ring	-0.0479	2	-0.0958	3	-0.1437	2	-0.0958	1	-0.0479
-OH aromatic	0.3496	0	0	0	0	0	0	0	0
-OH aliphatic	0.4617	4	1.8468	5	2.3085	2	0.9234	0	0
			6.9774		**9.8737**		**8.2062**		**3.267**

* F_i values adapted from [1].

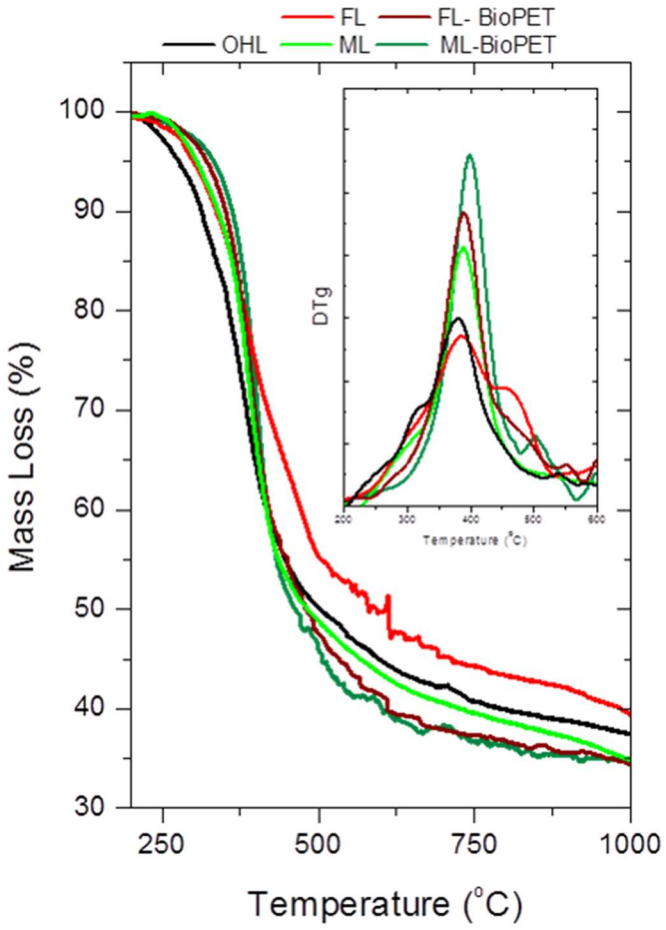

Figure S4: Mass Loss and derivative Mass in function of temperature for the lignins and blends

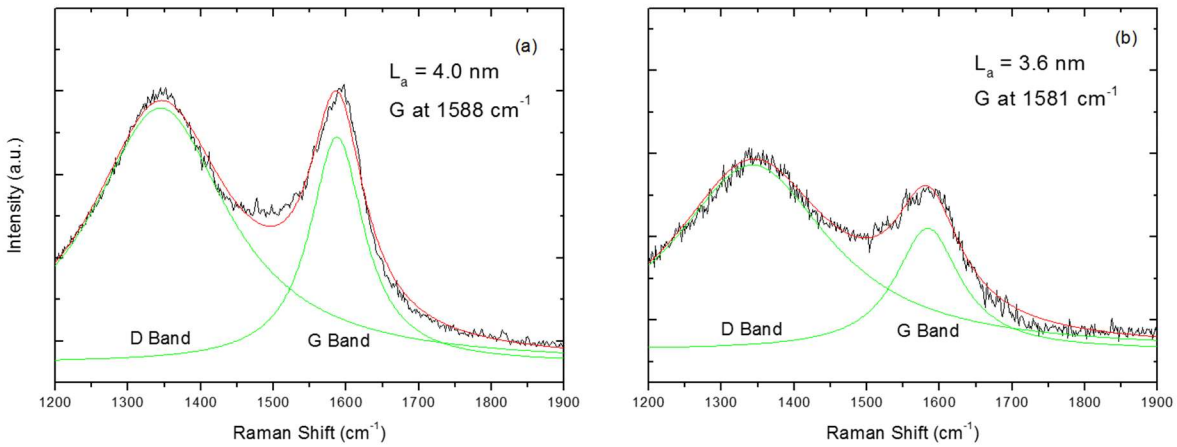

Figure S5: Raman spectra for 75%FL-25%BPET (a) and 75%ML-25% BPET (b). The D and G peaks (green) were deconvoluted using a Lorentz function. The sum of the 2 is marked in red.