Electronic supplementary information (ESI)

"Barking" up the right tree: biorefinery from waste stream to cyclic carbonate with immobilization of CO_2 for non-isocyanate polyurethanes

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1. Supplementary Tables

Table S1. Characteristics of the oxypropylation reaction and properties of HABO.

	HABO
Bark conversion rate (wt.%)	80
PO consumption (wt.%)[1]	87
Highest pressure reached (psi)[2]	470
Highest temperature reached (°C)	251
PO homopolymer content (wt.%)[3]	53
Oxypropylated bark macromolecules (wt.%)[3]	47

1. This value is estimated based on the final pressure after 2 h reaction, which is assumed to be only determined by unreacted vaporized PO;
2. This pressure value is also contributed by the N_2, which was used to fill the vessel initially (N_2 contributed about 88.5 psi at 251 °C);
3. HABO was subjected to an extraction using hexane under reflux to assess the ratio between the insoluble oxypropylated bark macromolecules and the soluble PO homopolymers.

Table S2. Characteristics and properties of the functionalized bark oils.

	HABO	Epox-HABO	Carb-HABO
Hydroxyl value (mg KOH)[1]	448.6	/	/
Epoxide equivalent weight (g/equiv)[2]	/	236.6	/
Carbonate content (wt.%)[3]	/	/	21.4
CO_2 fixed (wt.%)[3]	/	/	15.7
Viscosity (Pa·s)[4]	7	8	1500

1. Based upon the phthalic anhydride method as described in Method section,
2. Based upon ASTM D1652-11;
3. Detected by ^{1}H-NMR spectroscopy assuming no side reactions;
4. Measured with rheometer, shear rate = 1 s^{-1}, temperature = 25 °C.

Table S3 Chemical composition of tree bark from Western Red Cedar (all values were reported based upon the original bark weight).

Item	Extractives (Condensed tannin etc.) (wt.%)[1]	Klason Lignin (wt.%)[2]	Holocellulose (wt.%)[3]	α-cellulose (wt.%)[4]	Hemicellulose (wt.%)[5]	Ash content (wt.%)[6]
Bark	34.2 ± 2.2	15.0 ± 0.1	43.3 ± 0.3[4]	34.4 ± 0.5	8.9	3.3 ± 0.3

1. Experiment was carried out on bark raw materials according to *ASTM D1109-84. Standard Test Method for 1 % Sodium Hydroxide Solubility of Wood*;
2. Experiment was carried out on 1% NaOH extractives-free bark according to *Effland, M.J., 1977. Modified procedure to determine acid-insoluble lignin in wood and pulp. Tappi; (United States) 60:10*.
3. Experiment was carried out on 1% NaOH extractives-free bark according to *Wise, L., Murphy, M., Adieco, A.D., 1946. A chlorite holocellulose, its fractionation and bearing on summative wood analysis and studies on the hemicelluloses. Pap. Trade J. 122, 35–43*.
4. Experiment was conducted on obtained holocellulose according to *Browning, B., 1967. Methods of wood chemistry. Interscience / Wiley, New York*.
5. This result was obtained by subtracting the α-cellulose amount from holocellulose amount;
6. Experiment was conducted according to *ASTM D 1102-84. Standard Test Method for Ash in Wood*.

Table S4. TGA data of the crosslinked NIPU samples.

	T_{onset} (°C)	$T_{5\%}$ (°C)	$T_{30\%}$ (°C)	Ts (°C)	Residue @700 °C (%)
EDA1-1	224.0	221.4	282.4	126.4	15
EDA2-1	222.2	223.2	283.3	127.0	16
EDA1-2	196.6	201.4	264.4	117.2	18
HMDA1-1	193.5	210.6	304.2	130.7	16
IPDA1-1	220.9	230.0	310.9	136.5	14
DETA1-1	216.7	213.7	302.4	130.8	14
TAEA1-1	222.0	226.3	301.3	132.9	15

2. Supplementary Figures

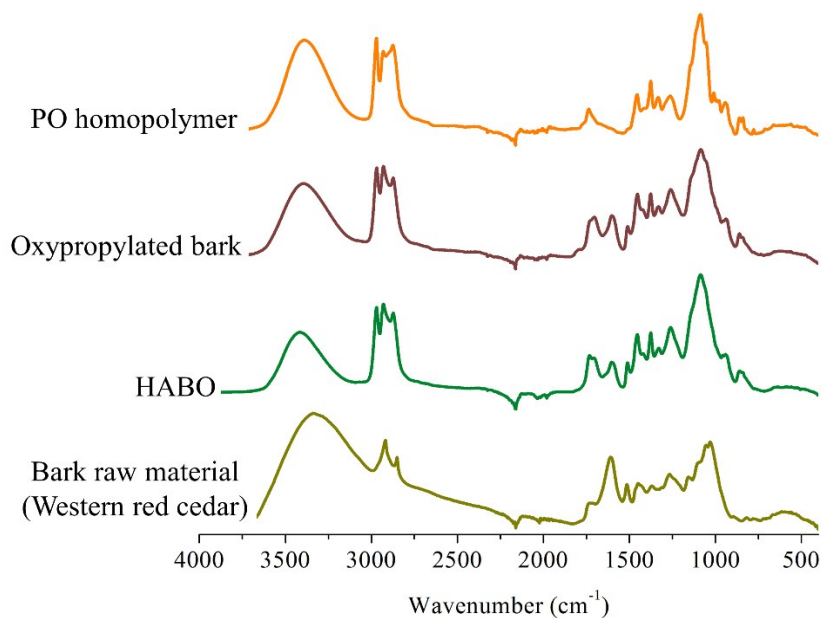Fig. S1. The change of temperature and pressure as a function of time for the bark oxypropylation process.

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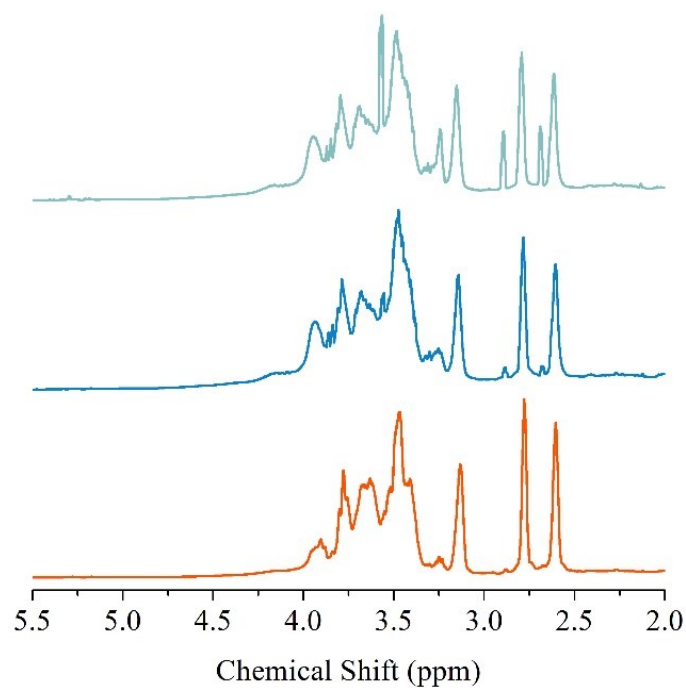
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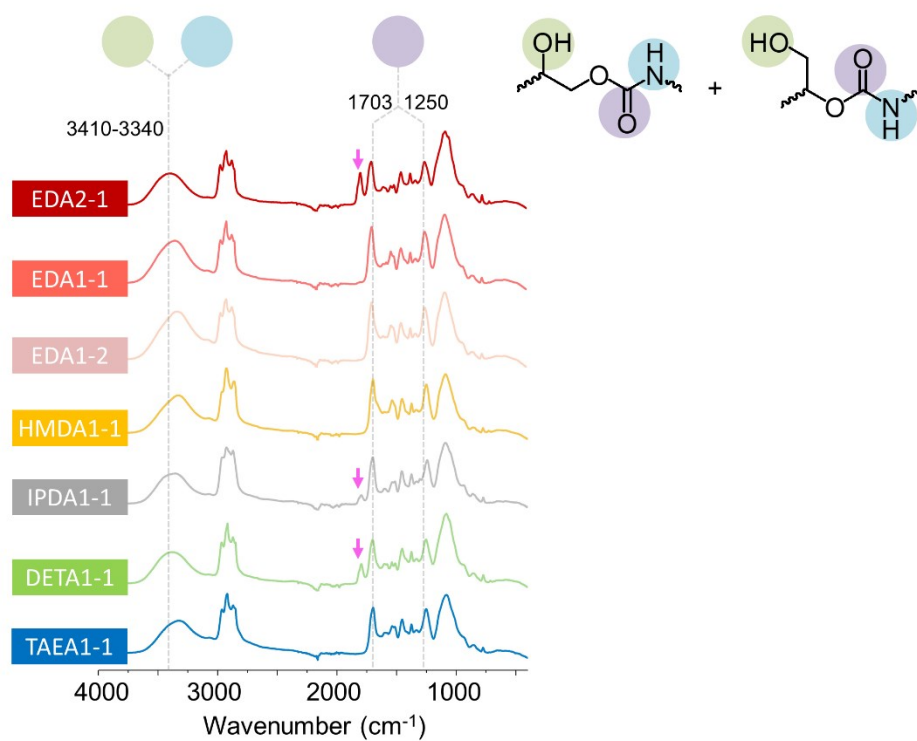

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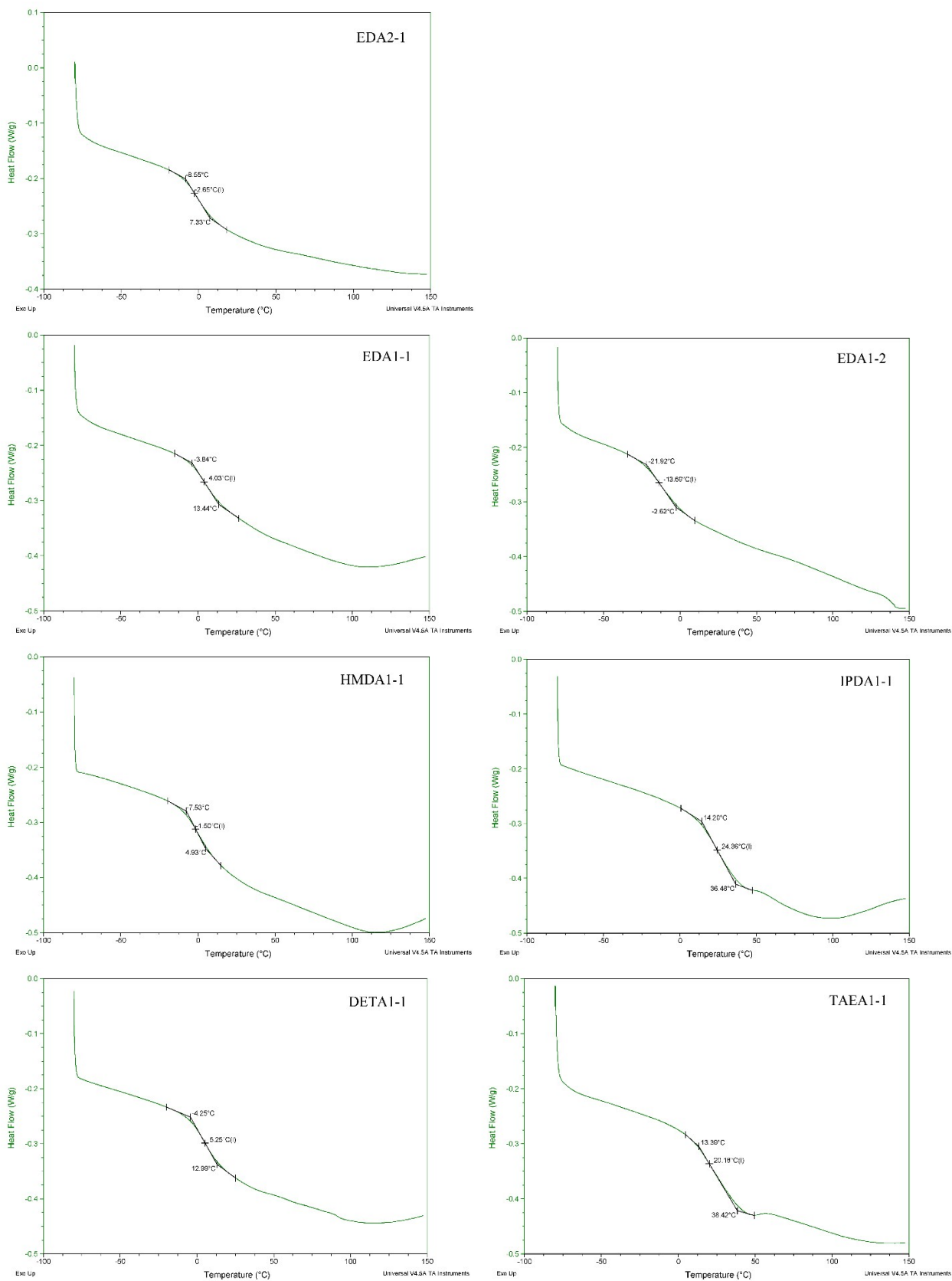
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