Supplementary Information (SI) for Green Chemistry.
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Supplementary material

Towards sustainable pulping of bagasse: silica migration, hexenuronic acid removal and ultrafiltration-based spent liquor utilization

Table S1 Applied analytics for the experimental work: **a** Bleaching-related samples; **b** Ultrafiltration-related samples; **c** Bleaching conditions and chemicals charge.

a Bleaching

Code (Sample)	Soxhlet and HPAEC-PAD	Paper sheets (optical properties)	GC-MS	UV-vis (HexA determination)	Fiber (kappa; viscosity; ISO)	SEM imaging	Fiber morphology (length; SEM-EDX; XRD; XPS)	ICP-OES
Fibrous bagasse (B)	×		×			×		×
Water treated bagasse (B-P1)	×		×			×		×
Alkali washed pulp (B-P1-P2)	×		×					×
Soda cooking pulp (B-P1-P2-C)	×	×	×	×	×	×	×	×
A/D_0	×	×	×	×	×			
A/D_0-E_p	×				×			
A/D_0-E_p-D_1	×	×			×			
D_0	×	×	×	×	×			
D_0-E_p	×				×			
D_0-E_p-D_1	×	×			×			

b Ultrafiltration

Code (Sample)	GC-MS	GPC	NMR	pH	Density	ICP-OES	Residual alkali
Feed	×			×	×	×	×
Feed lignin	×	×	×				
Permeate	×			×	×	×	×
Permeate lignin	×	×	×				
Retentate	×			×	×	×	×
Retentate lignin	×	×	×				

c Bleaching conditions and chemicals charge

Bleaching Sequence	Stage	T (℃)	t (min)	Const (%)	ClO_2 (%)	H_2SO_4 (%)	NaOH (%)	H_2O_2 (%)
D_0–Ep–D_1	D_0	55	40	10	3.2	0.3	-	-
	Ep	75	120	10	-	-	2.0	0.3
	D_1	75	180	10	2.0	-	-	-
A/D_0–Ep–D_1	A/D_0	90	140	10	2.0	0.7	-	-
	Ep	75	120	10	-	-	2.0	0.3
	D_1	75	180	10	2.0	-	-	-

Table S2. The quantitative profile of the crude extracts calculated based on the fibrous bagasse (B, **Table S1**): 1) dichloromethane (D) and 2) acetone (A) extractables of bagasse, and the 3) pretreated fraction of B-P1; as well as 4) B-P1-P2.

Code	Retention time, min	Compounds, detected as TMS ester/ether (TMS) derivatives	w/w, mg/g bagasse				MW	Characteristic fragments m/z	Databases
			D-B1	A-B1	B-P1	B-P1-P2			
1	7.168	Lactic acid (TMS ether; TMS ester)			0.17		23	219; 191; 147; 117; 73	[N]
2	7.637	Glycolic acid (TMS ether; TMS ester)			0.08	0.87	22	205; 177; 147; 73	[N]
3	9.647	Oxalic acid (TMS ether; TMS ester)				0.39	23	219; 190; 147; 73	[N]
4	9.988	Hydracrylic acid (TMS ether; TMS ester)				0.51	23	219; 177; 147; 73	[N]
5	14.614	1-Dimethylvinylsilyloxy-3-methylbenzene		0.03			19	192; 177	[N]
6	14.656	L-Isoleucine (N-TMS; TMS ester)			0.05		27	260; 232; 218; 158; 73	[N]
7	14.755	Phosphoric acid (tri TMS ether)				0.11	31	314; 299; 283; 211; 133; 73	[N]
8	15.052	Glycerol (tri TMS ether)		0.02	0.13	0.56	30	293; 218; 205; 147; 73	[N]
9	15.943	Succinic acid (di TMS ether)				0.099	26	262; 247; 147; 129; 73	[N]
10	16.82	Glyceric acid (diTMS ether; TMS ester)				0.19	32	307; 292; 205; 189; 147; 133; 103;	[N]
11	17.805	4-Hydroxybenzaldehyde	0.01	0.01		0.67	19	194; 179; 151	[N]
12	18.863	Tartronic acid (TMS ether, di TMS ester)				0.07	33	321; 292; 221; 147; 133; 102; 73	[N]; [A]
13	19.514	2,4-Dihydroxybutanoic acid (di TMS ether; TMS				0.31	33	321; 219; 203; 147; 129; 103; 73	[N]
14	20.175	3,4-Dihydroxybutanoic acid (di TMS ether; TMS				0.51	33	321; 233; 189; 147; 133; 117; 101;	[N]
15	21.989	Malic acid (TMS ether; di TMS ester)			0.07	0.13	35	335; 307; 245; 233; 147; 73	[N]
16	25.762	Phenylalanine (N-TMS; TMS ester)			0.03		30	294; 266; 218; 192; 147; 100; 73	[N]
17	25.8	L-Glutamic acid (N-TMS; diTMS ester)			0.09		36	363; 348; 246; 156; 147; 128; 73	[N]
18	26.349	Xyloisosaccharinic acid (XISA) (tri TMS ether; TMS ester)				0.011	438	423; 333; 321; 305; 231; 147; 103; 73	17
19	27.335	3-Deoxy-pentonic acid (tri TMS ether, TMS ester)				0.39	43	423; 335; 305; 245; 205; 147; 133;	17
20	27.376	3-Deoxy-pentaric acid (di TMS ether, di TMS ester)				0.11	452	437; 409; 379; 305; 245; 217; 147; 103; 73	17
21	31.462	citric acid (TMS ether; triTMS ester)			0.06		48	465; 375; 363; 347; 273; 147; 73	[N]
22	32.614	Quininic acid (quarTMS ether; TMS ester)				0.08	55	345; 255; 191; 147; 73	[N]
23	33.083	3-Hydroxy-3-(4-hydroxyphenyl) propanoic acid (diTMS ether; TMS ester)				0.09	398	398; 341; 267; 147; 73	[N]
24	33.448	Glucose (penta TMS ether)			0.07		54	435; 305; 217; 204; 191; 147; 129;	[N]
25	34.023	4-Coumaric acid (TMS ether; TMS ester)		0.17	0.24	5.544	30	308; 293; 249; 219	[N]

26	34.094	trans-Coniferryl alchool (di TMS ether)		0.02			32	324; 309; 293; 235; 204; 73	[N]
27	35.586	Methylpentadecanoic acid/C16:0 branched (TMS	0.01				32	328; 313; 145; 132; 117; 75; 73	[N]; [J]
28	35.735	Glucose (penta TMS ether)			0.10		54	435; 305; 217; 204; 191; 147; 129;	[N]
29	36.45	Palmitic acid/C16:0 (TMS ester)	0.05	0.04			32	328; 313; 145; 132; 117; 75; 73	[N]; [J];
30	37.453	Ferulic acid (TMS ether; TMS ester)				0.63	33	338; 323; 308; 249; 219; 73	[N]
31	37.555	trans-Sinapyl alcohol (di TMS ether)		0.01			35	354; 339; 323; 73	[N]
32	40.128	Linoleic acid (TMS ester)	0.00				35	352; 337; 262; 220; 150; 129; 117;	[N];
33	40.252	Oleic acid (TMS ester)	0.02	0.01			35	354; 339; 264; 222; 199; 145; 129;	[N]; [A]
34	40.83	Stearic acid/C18:0 (TMS ester)	0.02	0.01			35	356; 341; 145; 132; 129; 117; 75; 73	[N]; [J];
35	44.884	Arachidic acid/C20:0 (TMS ester)	0.01	0.01			38	384; 369; 145; 132; 129; 117; 75	[N]
36	47.974	1-Monopalmitin (di TMS ether)	0.01				47	459; 371; 239; 205; 147; 129; 73	[N]
37	48.645	Behenic acid/C22:0 (TMS ester)	0.01	0.00			41	412; 397; 145; 132; 129; 117; 75; 73	[N]
38	49.682	Sucrose (nona TMS ether)				0.71	91	451; 437; 361	[N]
39	51.563	Trehalose (nona TMS ether)			1.22	0.14	91	451; 437; 361	[A]
40	52.16	Lignoceric acid/C24:0 (TMS ester)	0.01	0.01			44	440; 425; 145; 132; 129; 117; 73	[N]
41	53.965	1-Hexacosanol (TMS ether)	0.02				45	439; 75	[N]
42	55.443	hexacosanoic acid/ C26:0 (TMS ester)		0.01			46	468; 453; 145; 132; 129; 117	[N]
43	57.175	1-Octacosanol (TMS ether)	0.17	0.01			48	467; 75	[N]
44	58.552	Octacosanoic acid / C28:0 (TMS ester)	0.01	0.03			49	496; 481; 145; 132; 117	[N]
45	58.992	Campesterol (TMS ether)	0.03				47	472; 457; 382; 367; 343; 255; 129;	[N]
46	59.474	Stigmasterol (TMS ether)	0.03				48	484; 469; 394; 379; 351; 255; 129	[N]
47	60.102	1-Triacontanol (TMS ether)	0.02				51	495; 75	[N]
48	60.348	β-Sitosterol (TMS ether)	0.06				48	486; 471; 396; 381; 357; 129; 73	[N]; [A]
49	61.599	Triacontanoic acid/ C30:0 (TMS ester)		0.01			52	524; 509; 201; 145; 132; 129; 117	[N]

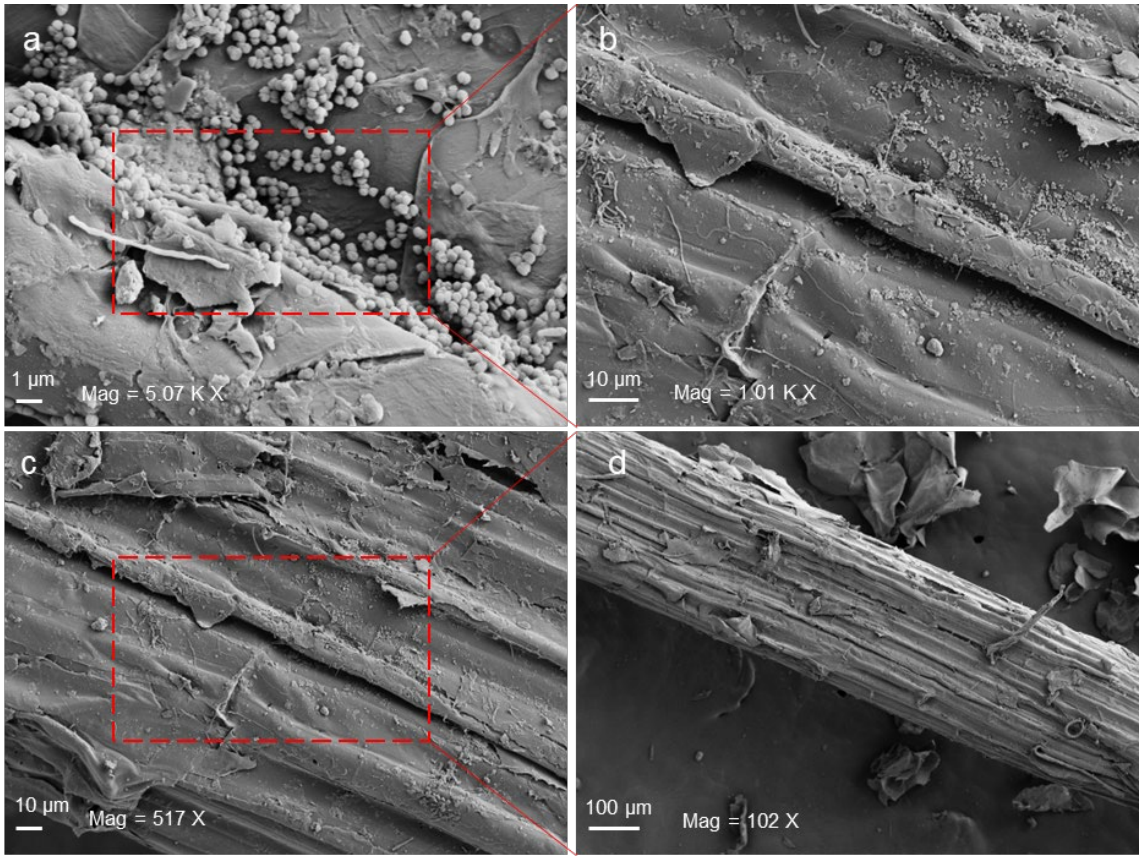


Fig. S1 SEM imaging at the increasing magnification (a->d) of fibrous bagasse B (**Table S1**)

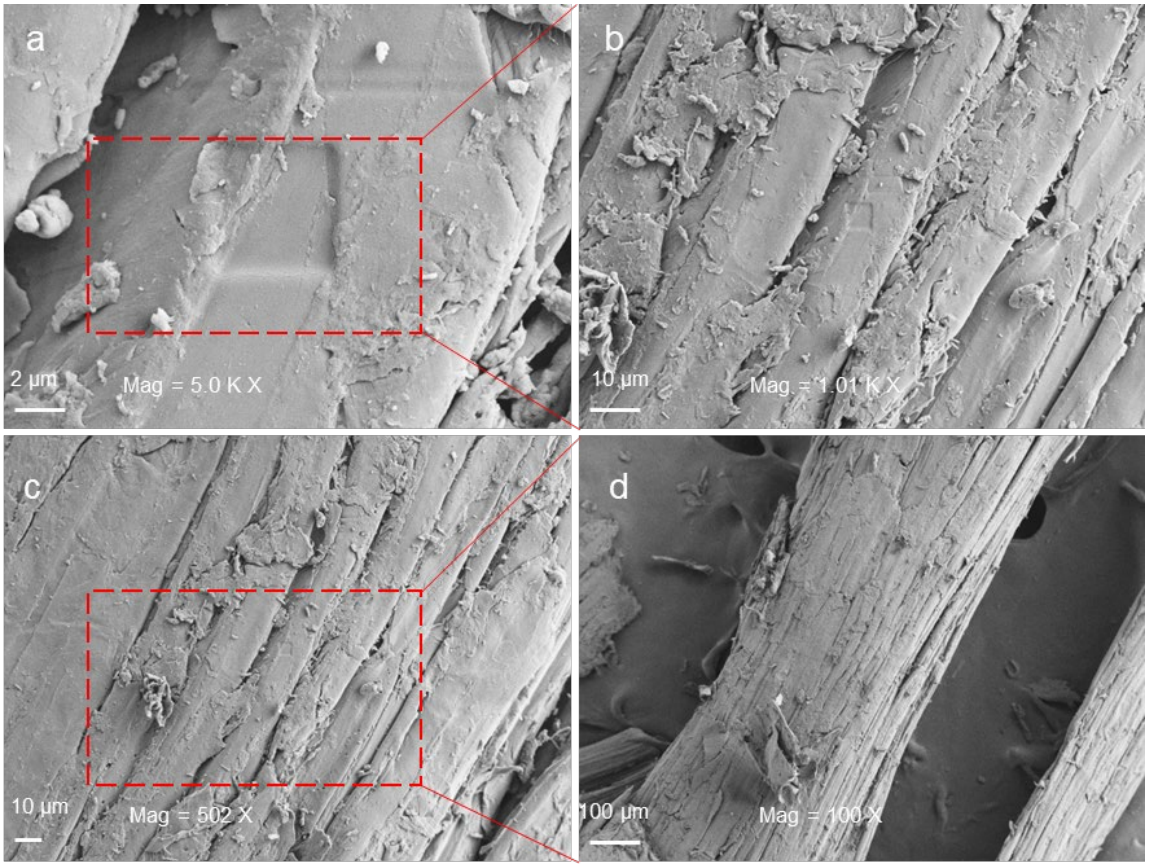


Fig. S2 SEM imaging at increasing magnification (a->d) of hot water-washed bagasse (B-P1) (**Table S1**)

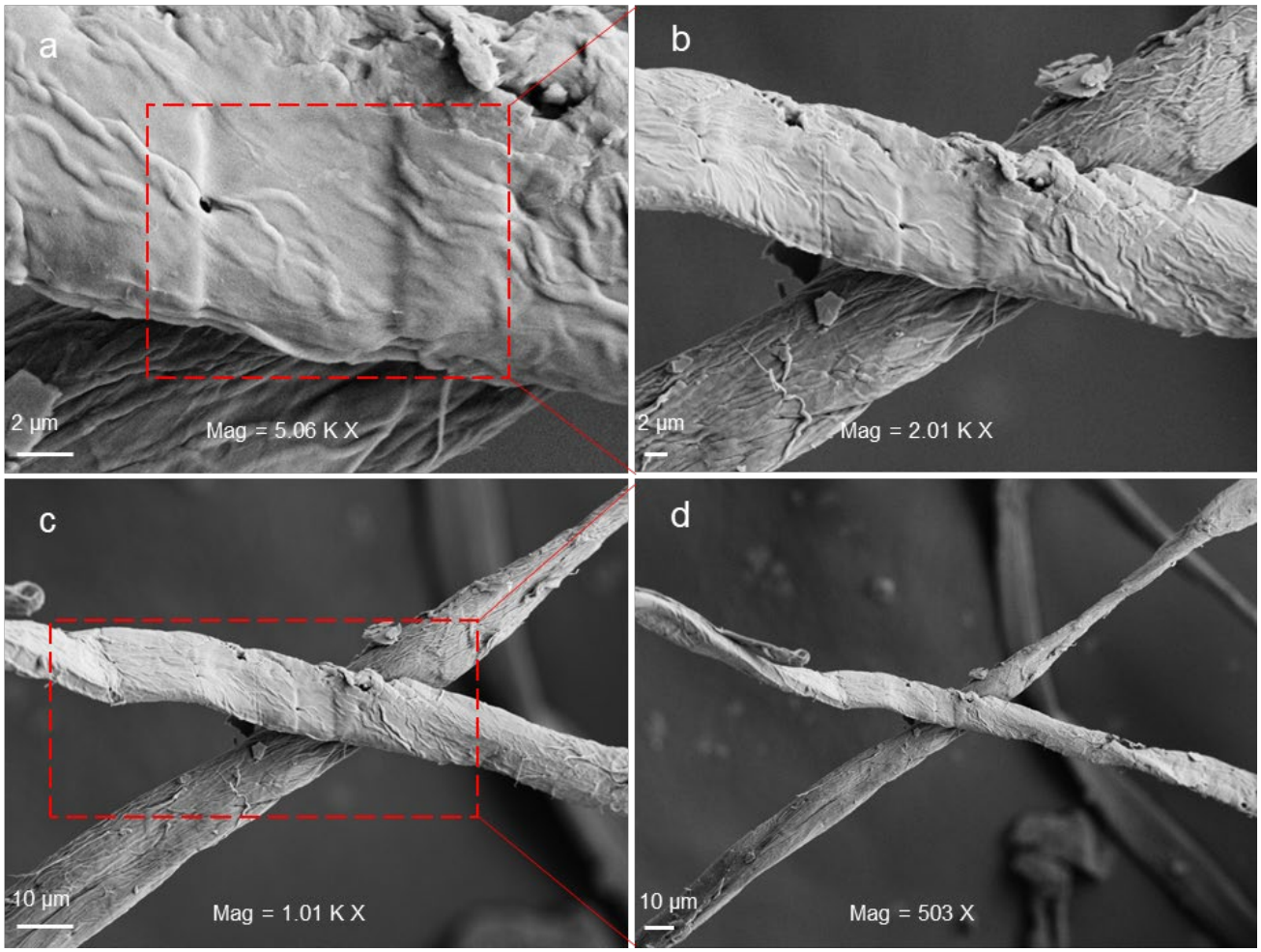
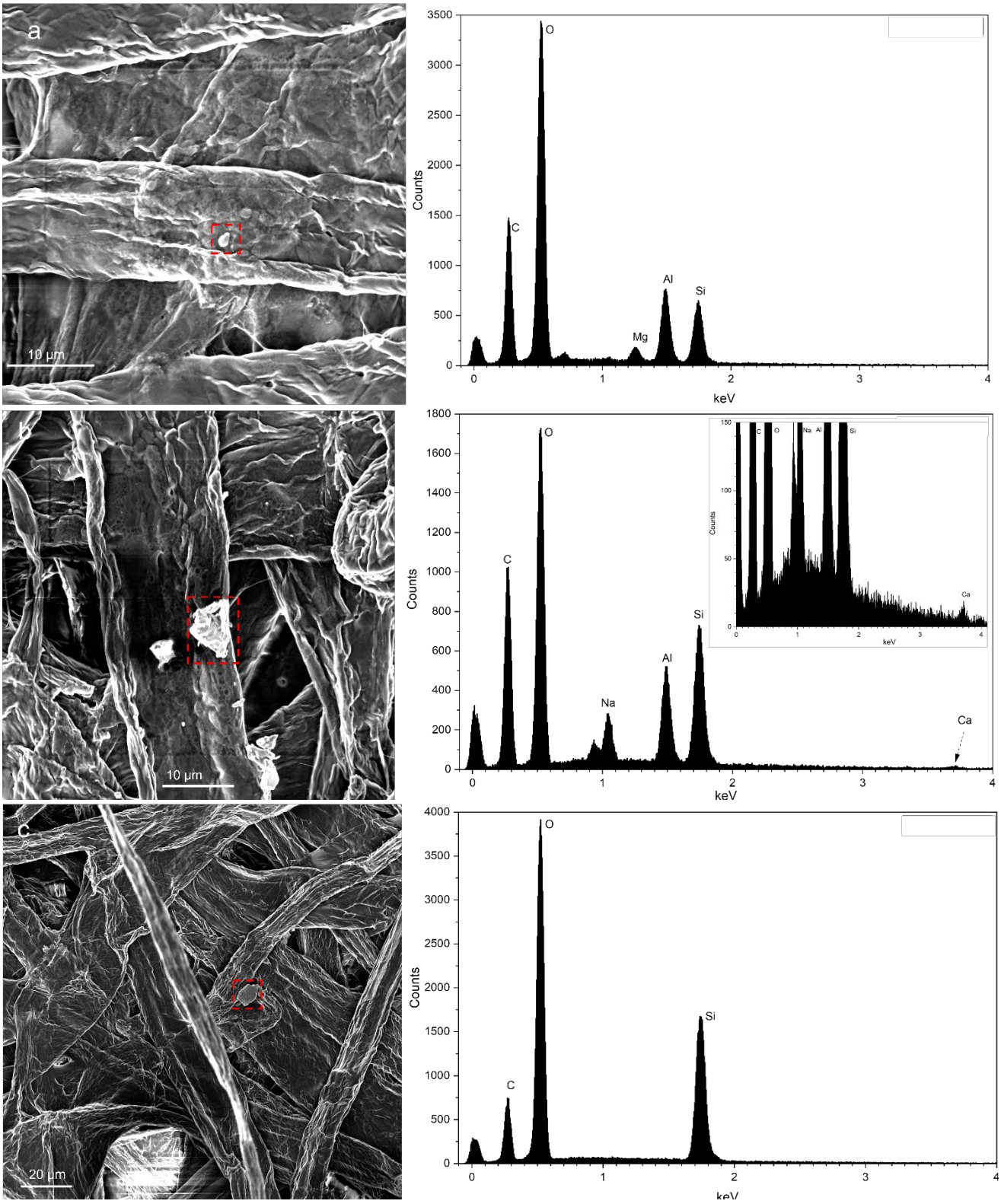
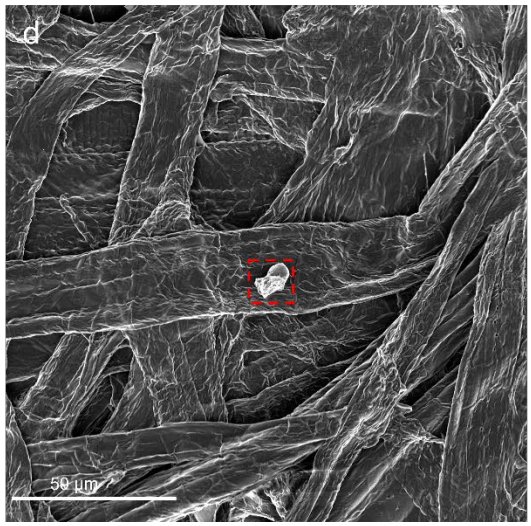


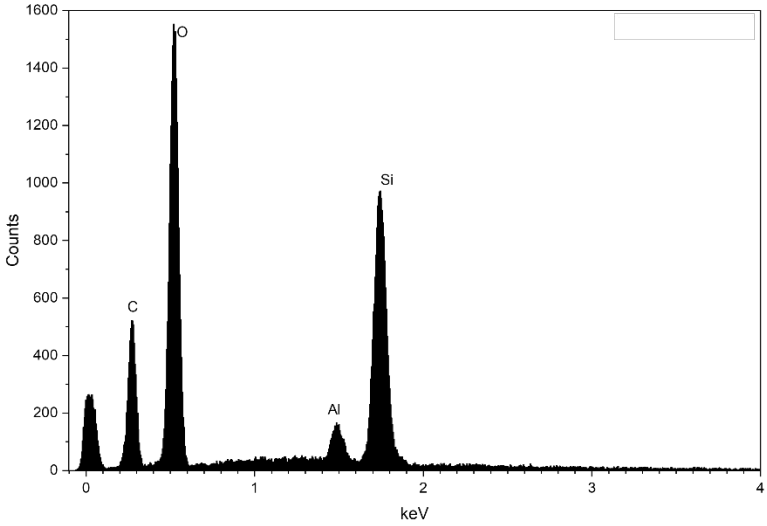
Fig. S3 SEM imaging at increasing magnification (a->d) of cooked pulp (B-P1-P2-C) (**Table S1**)

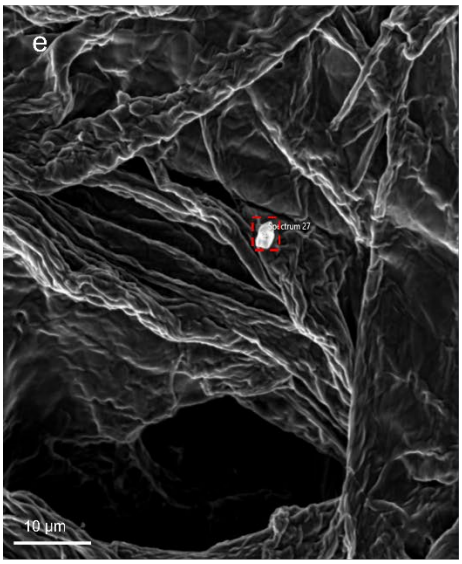
Table S3 Fiber morphology acquisition from Valmet Fiber Image Analyser FS 5.

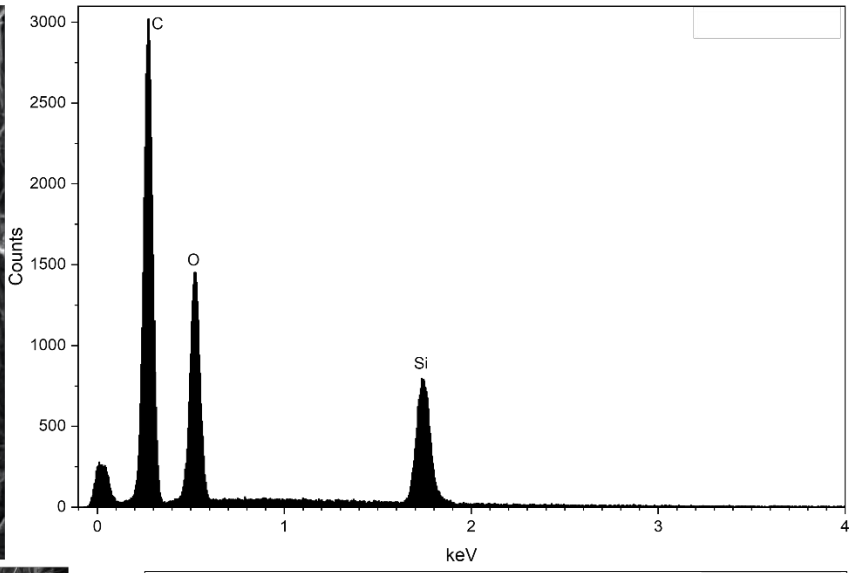
Codes	Full name	Number	Unit
Lc(n) [mm]	Arithmetic average fiber length	0.501	mm
Lc(l) [mm]	Length-weighted fiber length	0.992	mm
Lc(w) [mm]	Weight-weighted average fiber length	1.645	mm
Lc(n) ISO [mm]		0.638	mm
Lc(l) ISO [mm]		1.067	mm
Lc(w) ISO [mm]		1.663	mm
Fiber width [µm]	Width	21.02	um
Aspect ratio		47	
Aspect ratio (ISO)		51	
Curl %		7.93	%

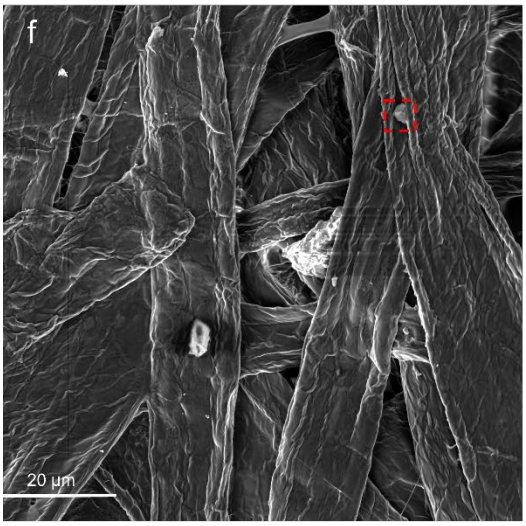

a
10 µm
Counts
keV
O
C
Mg
Al
Si
b
10 µm
Counts
keV
O
C
Na
Al
Si
Ca
c
20 µm
Counts
keV
O
C
Si

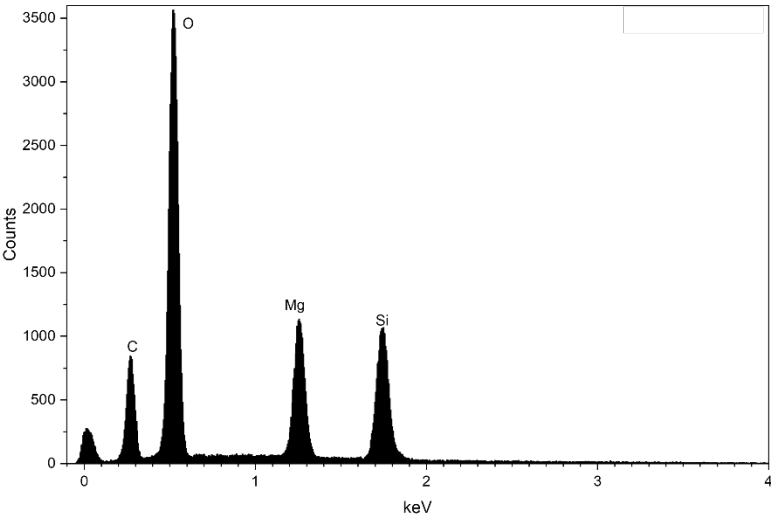

d
50 µm


O
Si
C
Al
Counts
keV


e
10 µm


C
O
Si
Counts
keV


f
20 µm


O
Mg
Si
C
Counts
keV

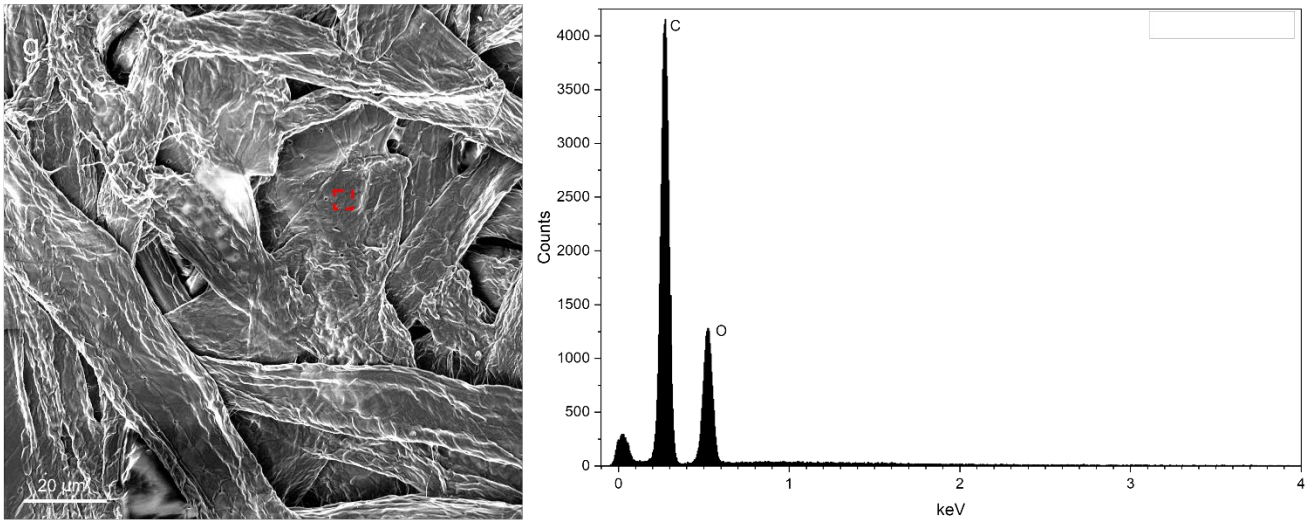


Fig. S4 SEM-EDX analysis of bagasse B-P1-P2-C pulp sheet fibers based on six spectrum positions (highlighted in red dashed rectangle) in comparison to reference pulp cellulose fiber (**g**): **a** Spectrum 1 (primary form being aluminosilicate); **b** Spectrum 2 (calcium silicate); **c** Spectrum 3 (silicon dioxide); **d** Spectrum 4 (silicon dioxide); **e** Spectrum 5 (silicon dioxide); **f** Spectrum 6 (magnesium silicates); **g** reference (pulp cellulose fiber).

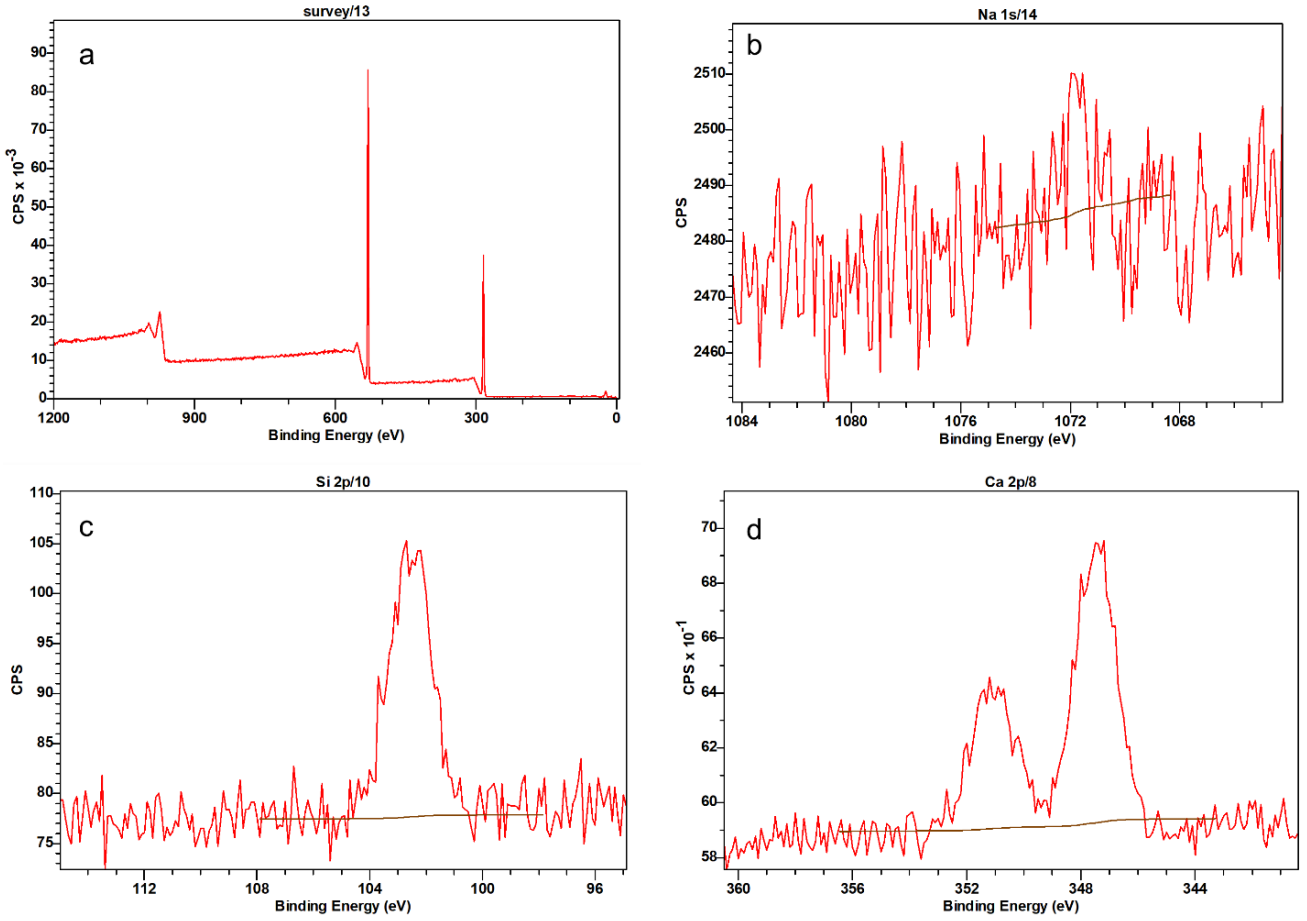


Fig. S5 XPS spectra shows wide-range surveys scan (**a**) as well as high-resolution spectra from the Na 1s (**b**), Si 2p (**c**), and Ca 2p (**d**) regions from the sample B-P1-P2-C (post-extracted).

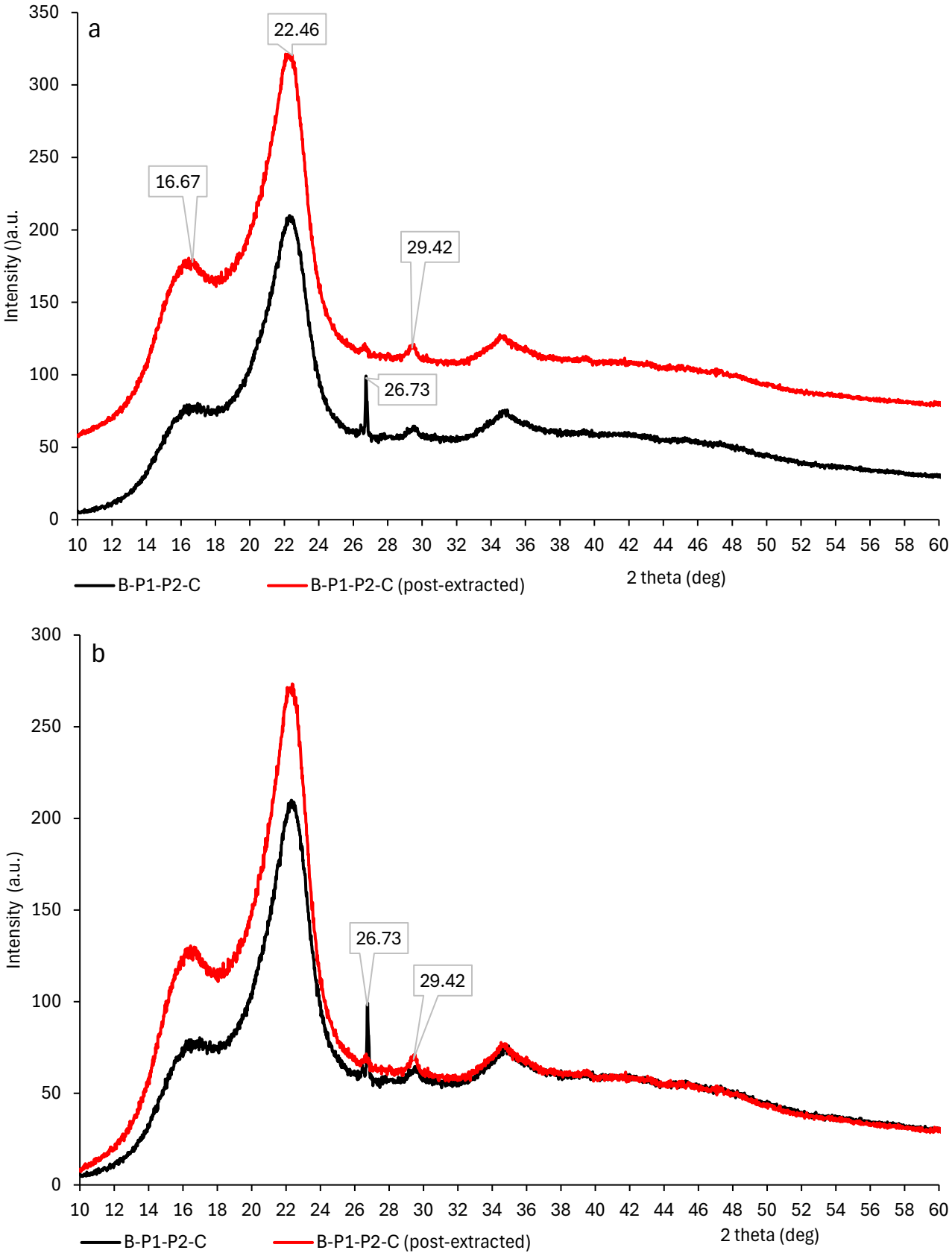


Fig. S6 XRD patterns of B-P1-P2-C sample in comparison to its post-extracted form (B-P1-P2-C (post-extracted)) in different forms: **a** stacked plot; **b** layer by layer.

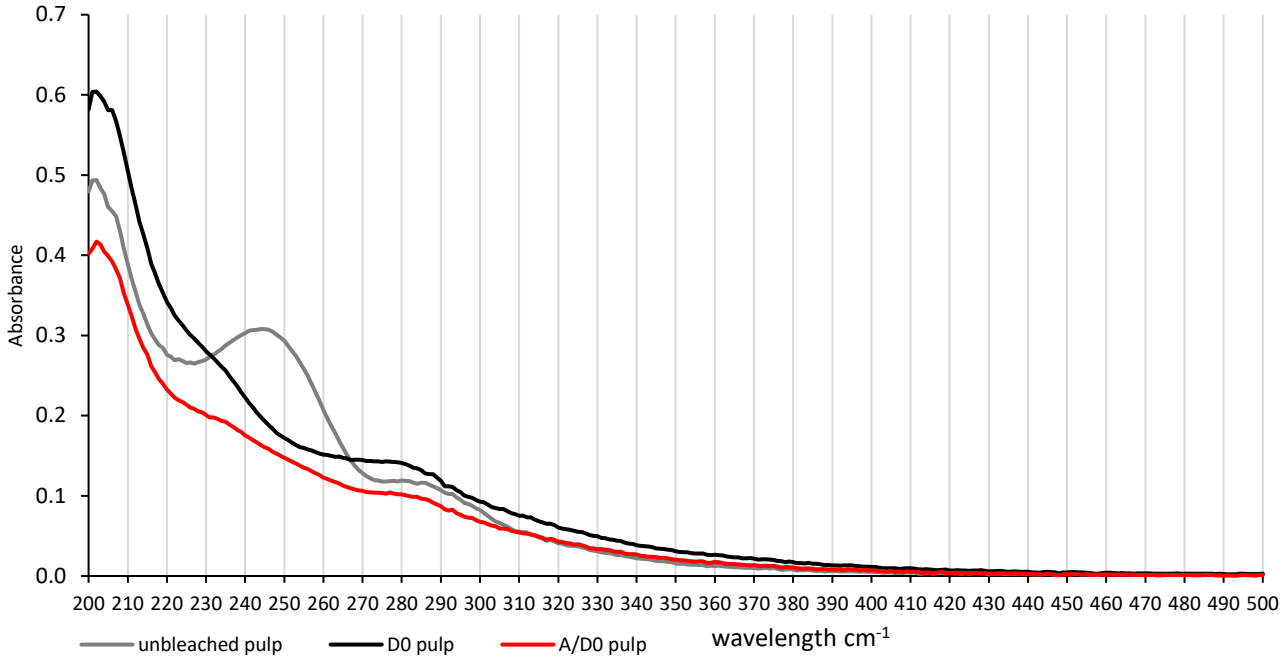


Fig. S7 UV-vis spectrum of the acid hydrolysate from multiple sources of the pulp: 1) unbleached pulp (B-P1-P2-C); 2) D_0 pulp; 3) A/D_0 pulp. See **Table S1** for the abbreviations.

Table S4 Preparation of GC-MS total-ion chromatogram of B-P1-P2 along with the A/D0 and DO hydrolysate. Hydrolysate amount differs from 400g (B-P1-P2-1; B-P1-P2-C-A/D0-1; B-P1-P2-C-A/D0-2; B-P1-P2-C-D0-1) to 50 or 100g depending on the sample source. 2-Furonic acid (2-FA) is calculated semi-quantitatively based on the relative intensities' ratios between 2-FA/ C24.

		pulp,g	splatted / overall hydrolysate, g	Evaporated solid, mg	Intensity C24	Intensity 2-furonic acid (2-FA)	2-FA/ pulp; mg/g	Average of 2-FA/ pulp; mg/g (std)
B-P1-P2	B-P1-P2-1	3.7	400.3/1529.3	28.7	90881623	130957470	0.73	0.59 (0.11)
	B-P1-P2-2	3.7	99.8/1529.3	2.49	105116411	29247917	0.57	
	B-P1-P2-3	3.7	100.3/1529.3	2.3	105413007	23626233	0.46	
	B-P1-P2-4	3.7	100.0/ 1529.3	3.15	109033808	31342294	0.59	
B-P1-P2-C-A/D0	B-P1-P2-C-A/D0-1	1.5	399.9/ 599.9	26.3	92726655	29734050	0.16	0.14 (0.04)
	B-P1-P2-C-A/D0-2	3.7	397.3/ 1499.4	25.1	95346840	32218004	0.17	
	B-P1-P2-C-A/D0-3	1.5	51.2/ 599.9	1.29	107703820	5647115	0.21	
	B-P1-P2-C-A/D0-4	3.7	100.4/ 1499.4	3.15	112709033	5913800	0.10	
	B-P1-P2-C-A/D0-5	3.7	100.2/ 1499.4	3.21	111185545	6449772	0.12	
	B-P1-P2-C-A/D0-6	3.7	99.9/ 1499.4	3.07	110449214	5907132	0.11	
B-P1-P2-C-D0	B-P1-P2-C-D0-1	1.5	399.6/ 604.5	33.6	93087322	14181323	0.08	0.05 (0.02)
	B-P1-P2-C-D0-2	1.5	49.8/ 604.5	2.15	109739423	1472416	0.05	
	B-P1-P2-C-D0-3	1.5	49.8/ 604.5	1.39	112353926	849316	0.03	

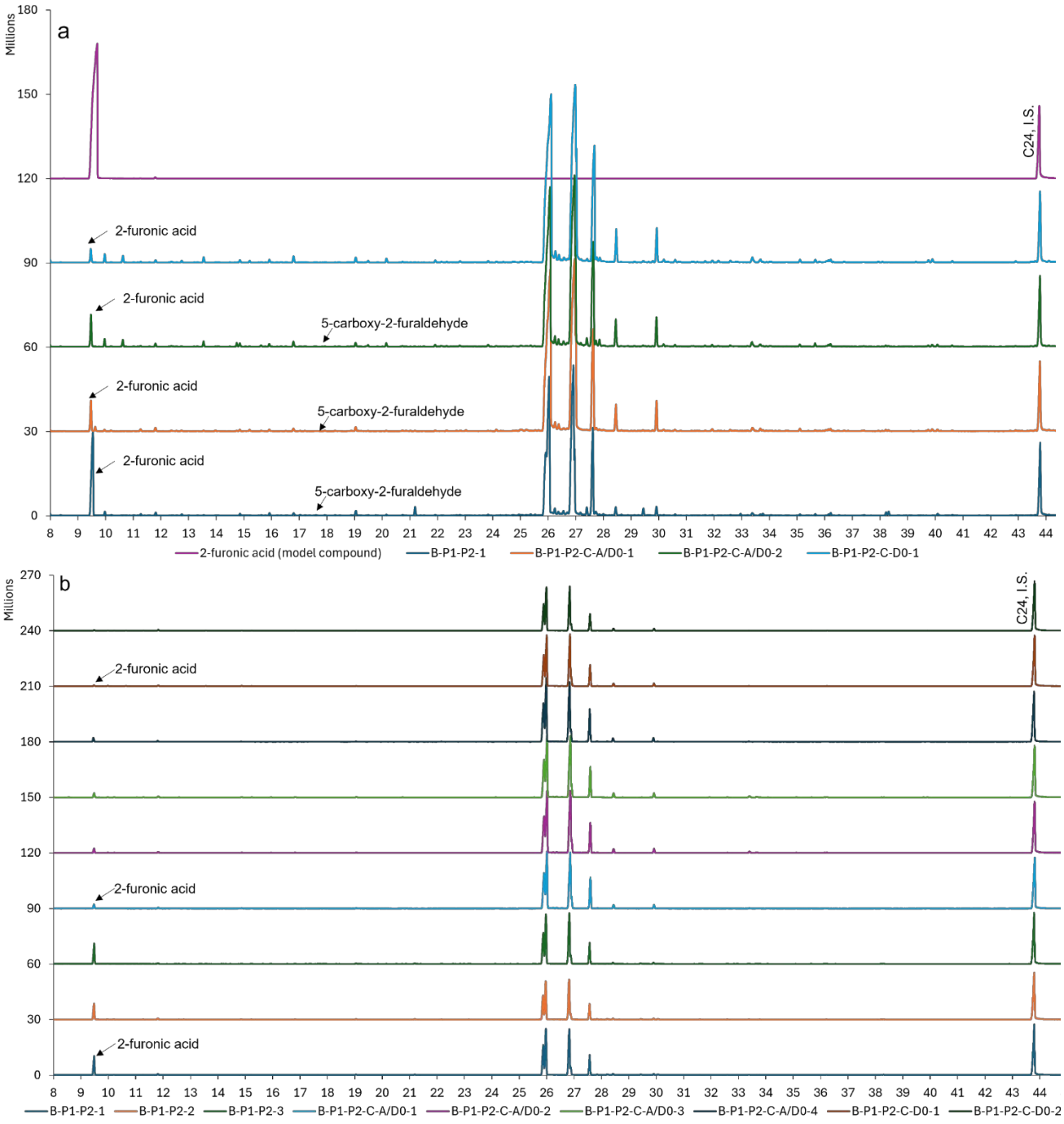


Fig. S8 GC-MS total-ion chromatogram of B-P1-P2 along with the A-D0 and D0 hydrolysate showing major peaks for: 2-furonic acid (2-furancarboxylic acid; CAS 88-14-2), 5-formyl-2-furancarboxylic acid (5-carboxy-2-furaldehyde; CAS 13529-17-4) and internal standard (C24, i.s.): **a** hydrolysate amount being 400g; **b** hydrolysate amount being 50 or 100g.

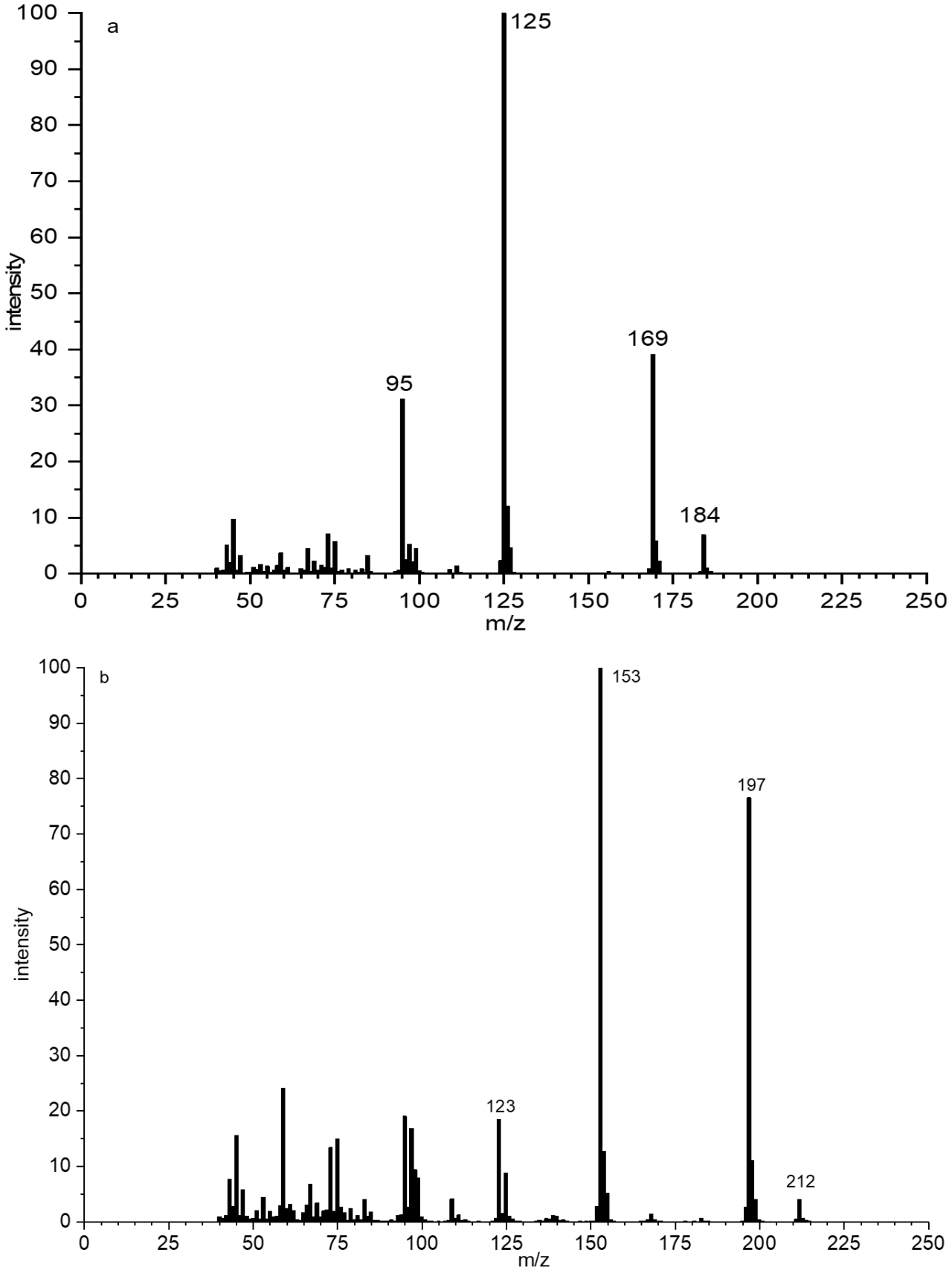


Fig. S9 mass spectrum of the degradation products of HexA: **a** 2-furonic acid (2-furancarboxylic Acid; CAS 88-14-2); **b** 5-formyl-2-furancarboxylic acid (5-carboxy-2-furaldehyde; CAS 13529)

Table S5 Overall chemical composition (a) and carbohydrate composition (b) (% of anhydrosugars in the original dry mass without yield consideration) from the fibrous bagasse (B, **Table S1**) to the bleached pulp.

a

	Sugar	Lignin	Extractives
B	56.5 (1.1)	25.78 (0.2)	0.26
B-P1	47.4 (0.9)	23.84 (0.6)	0.09
B-P1-P2	71.58 (1.3)	22.62 (0.3)	0.20
B-P1-P2-C	94.82 (0.7)	1.40 (0.1)	0.13
A/D_0	95.95 (0.7)	0.97 (0.01)	0.13
A/D_0-E_p	95.57 (1.2)	0.95 (0.1)	0.06
A/D_0-E_p-D_1	95.79 (0.8)	0.86 (0.03)	0.08
D0	96.20 (0.9)	1.05 (0.1)	0.13
D_0-E_p	91.50 (0.9)	1.05 (0.005)	0.11
D_0-E_p-D_1	92.25 (0.1)	0.88 (0.1)	0.06

b

	Ara	Rha	Gal	Glc	Xyl	Man
B	1.9 (0.2)	0	0.5 (0.1)	34.8 (0.2)	19.4 (0.2)	0
B-P1	1.7 (0.1)	0	0.5 (0.1)	39.5 (0.4)	21.6 (0.6)	0
B-P1-P2	2.0 (0.2)	0	0.4 (0.1)	45.0 (0.4)	24.2 (0.6)	0
B-P1-P2-C	1.6 (0.1)	0	0	68.8 (0.5)	24.5 (0.6)	0
A/D_0	1.1 (0.01)	0	0	70.3 (0.9)	24.6 (0.2)	0
A/D_0-E_p	1.1 (0.1)	0	0	70.9 (0.3)	23.6 (0.3)	0
A/D_0-E_p-D_1	0.4 (0.2)	0	0	71.6 (0.5)	23.9 (0.5)	0
D_0	1.5 (0.1)	0	0	70.1 (0.7)	24.7 (0.2)	0
D_0-E_p	1.4 (0.1)	0	0	66.3 (0.8)	23.9 (0.1)	0
D_0-E_p-D_1	0.6 (0.1)	0	0	67.5 (0.6)	24.2 (0.3)	0

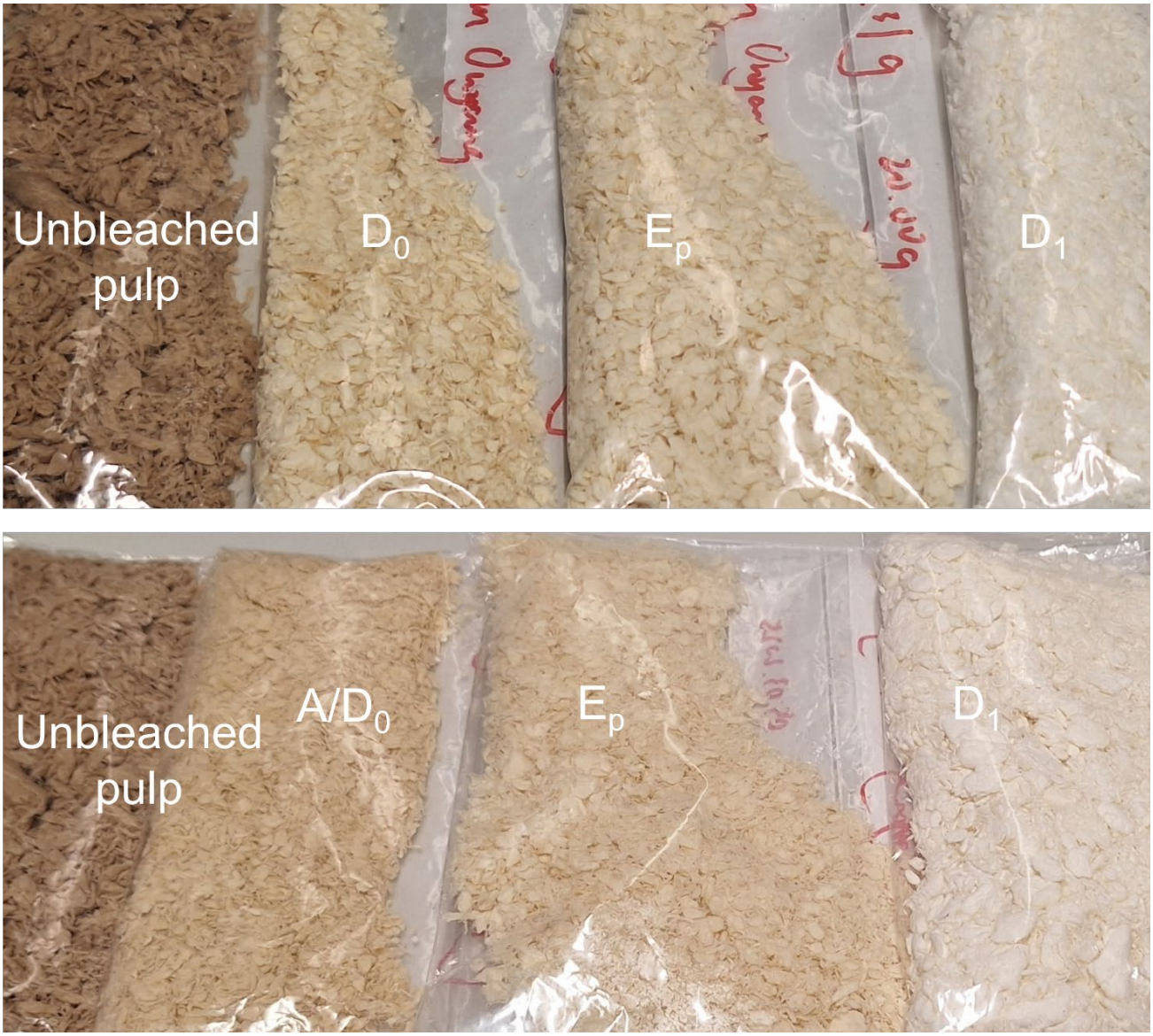


Fig. S10 Photograph of the pulp comparison between the D_0-E_p-D_1 and A/D_0-E_p-D_1.

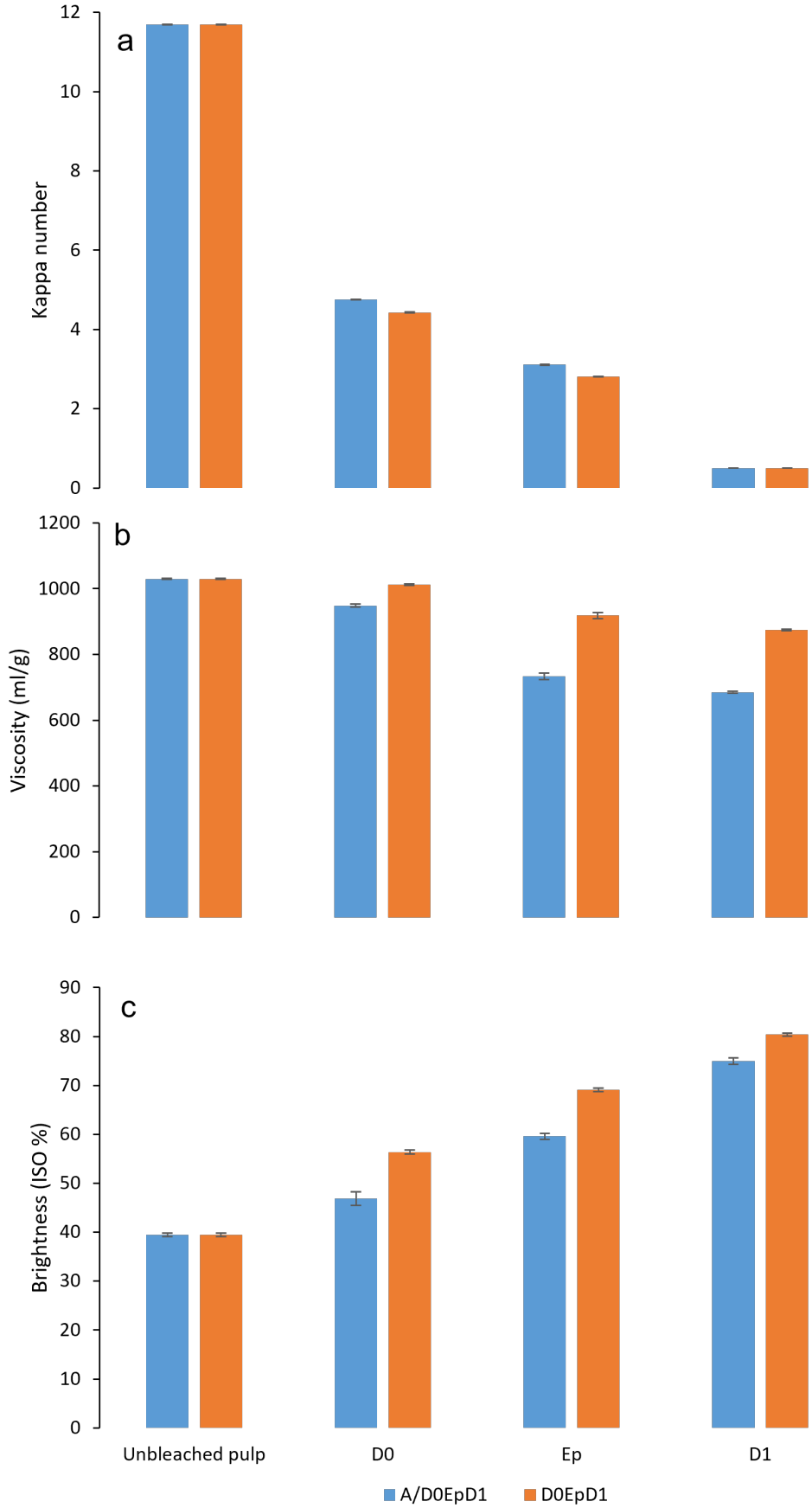


Fig. S11 Pulps' properties of bagasse delignified pulp treated with A/$D_0E_pD_1$ (5.2 %Act. Cl), in comparison to $D_0E_pD_1$ (4%Act. Cl): **a** Kappa; **b** Viscosity; **c** ISO brightness.

Table S6 Their exact datapoints and basic profile properties of the paper sheets (optical properties). Standard deviations are included as part of parenthesis.

	Tensile properties			Profile of sheet			
	Tensile strength (kN/m)	Young´s Modulus (Gpa)	Tensile index (Nm/g)	Thickness (mm)	Density (kg/m^3)	Mass of one sheet (g)	Grammage (g/ m^2)
B-P1-P2-C	7.999 (0.341)	1.814 (0.135)	41.924 (1.788)	0.305 (0.021)	625.6	0.1431	190.8
D0	7.512 (0.205)	1.592 (0.122)	28.88 (0.788)	0.408 (0.106)	637.5	0.1951	260.1
A/D0	7.874 (0.272)	1.681 (0.073)	27.559 (0.952)	0.381 (0.071)	749.8	0.2143	285.7
D0-Ep-D1 (sheet 1)	9.586 (0.415)	1.882 (0.07)	32.538 (1.407)	0.425 (0.049)	693.1	0.2209	294.6
D0-Ep-D1 (sheet 2)	9.225 (0.369)	1.594 (0.125)	28.359 (1.134)	0.432 (0.059)	753.1	0.2440	325.3
A/D0-Ep-D1 (sheet 1)	9.225 (0.765)	1.739 (0.044)	26.321 (2.183)	0.471 (0.083)	744.1	0.2629	350.5
A/D0-Ep-D1 (sheet 2)	7.498 (1.1)	1.89 (0.332)	26.912 (3.948)	0.367 (0.047)	759.2	0.2090	278.6

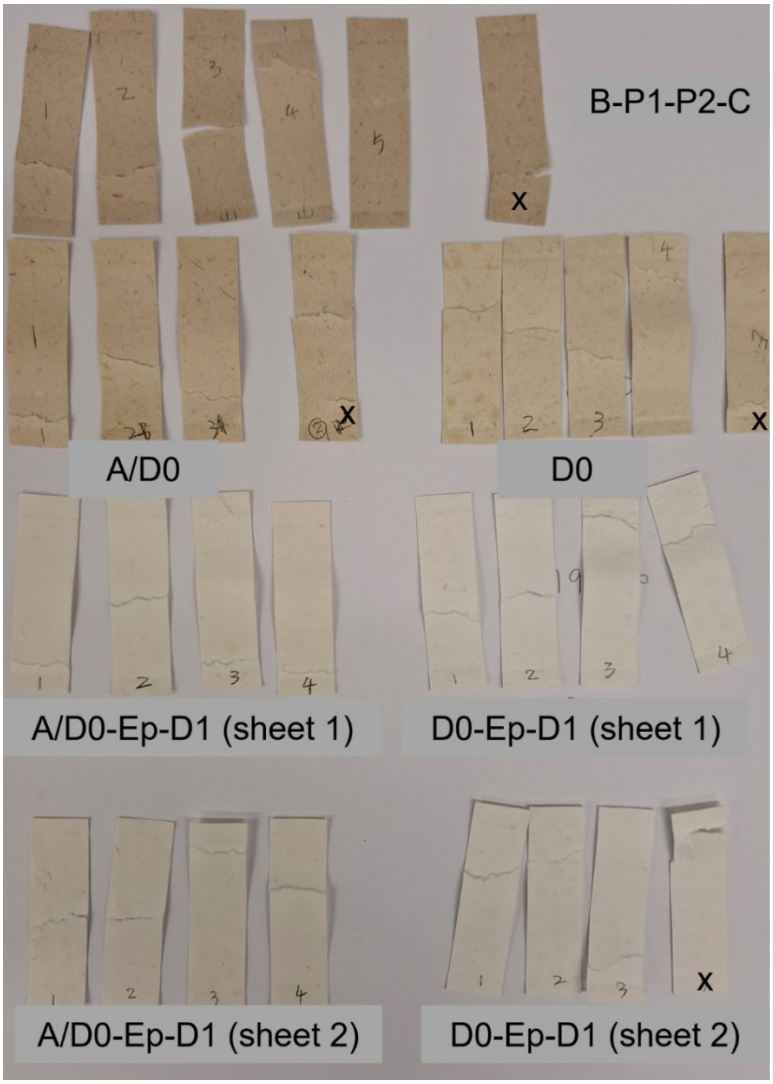
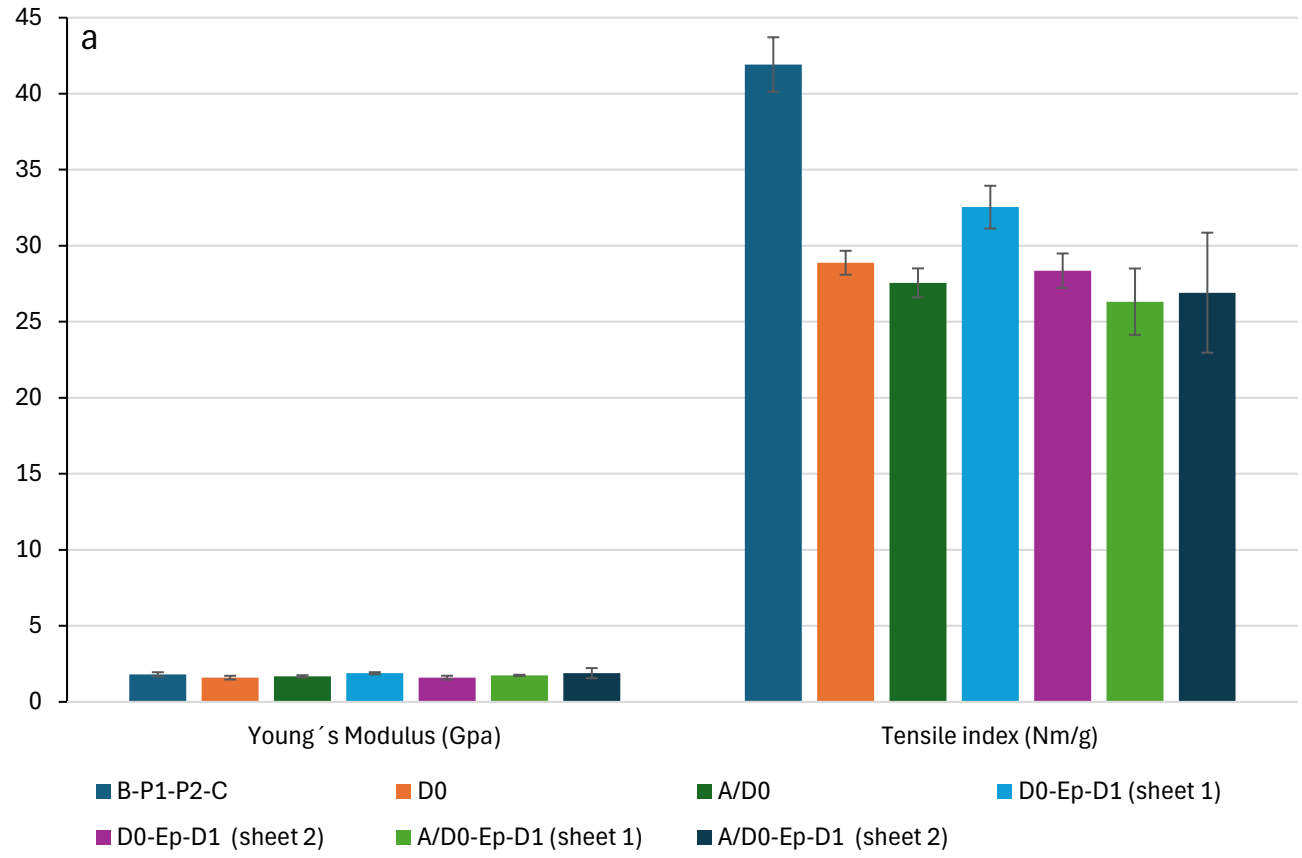


Fig. S12 Photograph of the fracture surface of laboratory paper sheets (optical properties) after the tensile test.



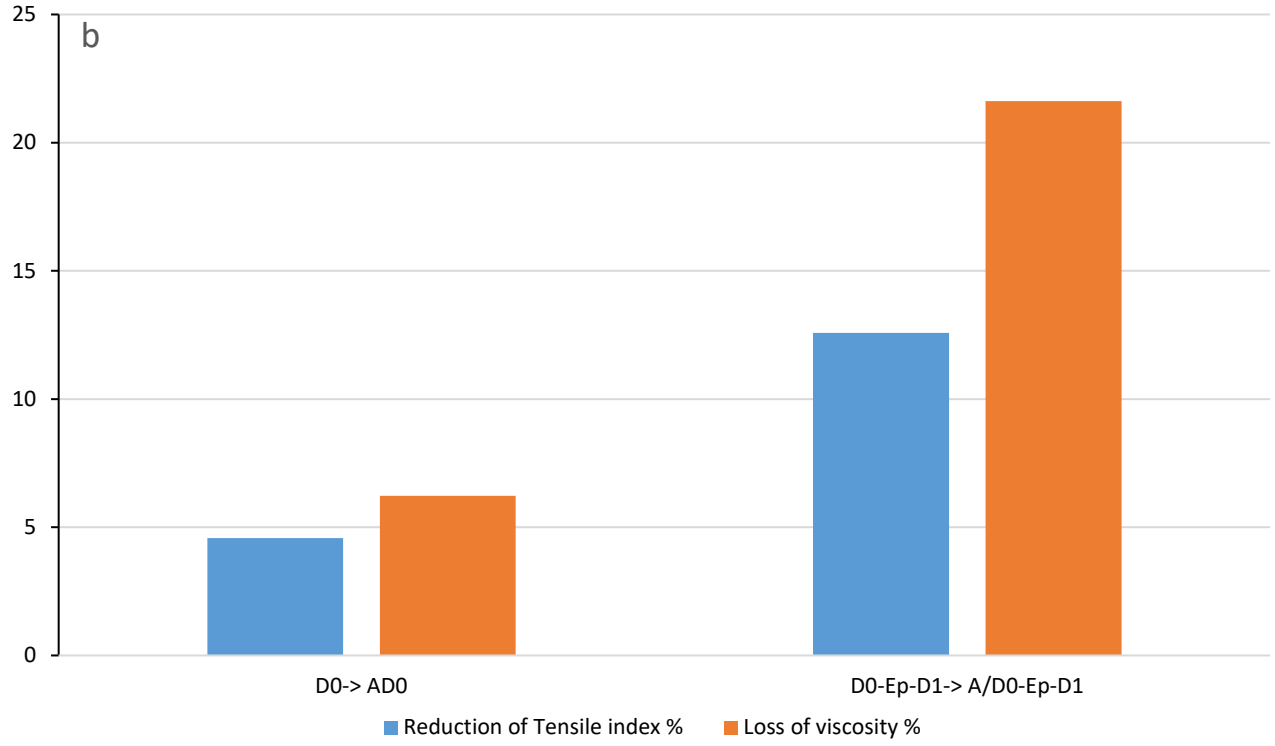
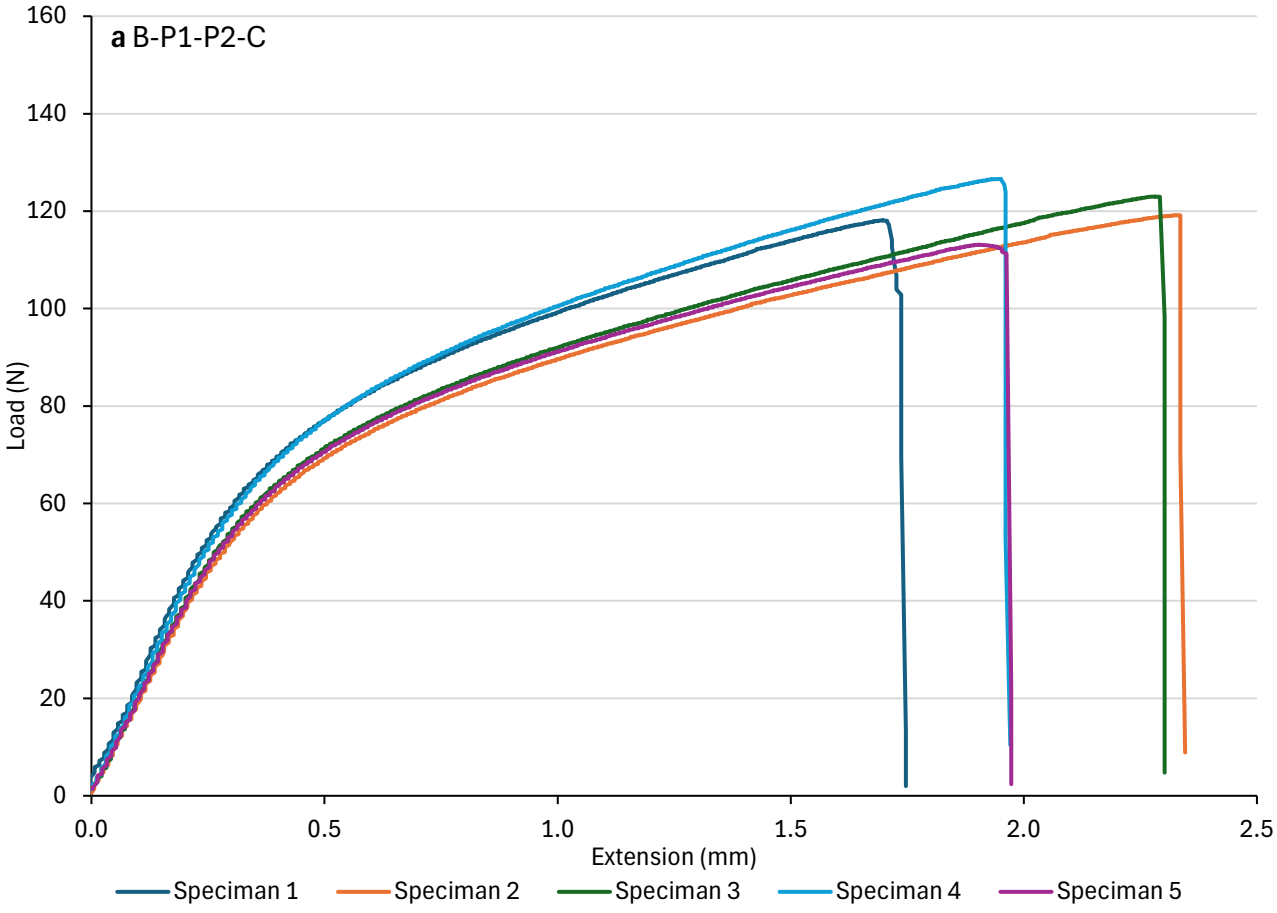
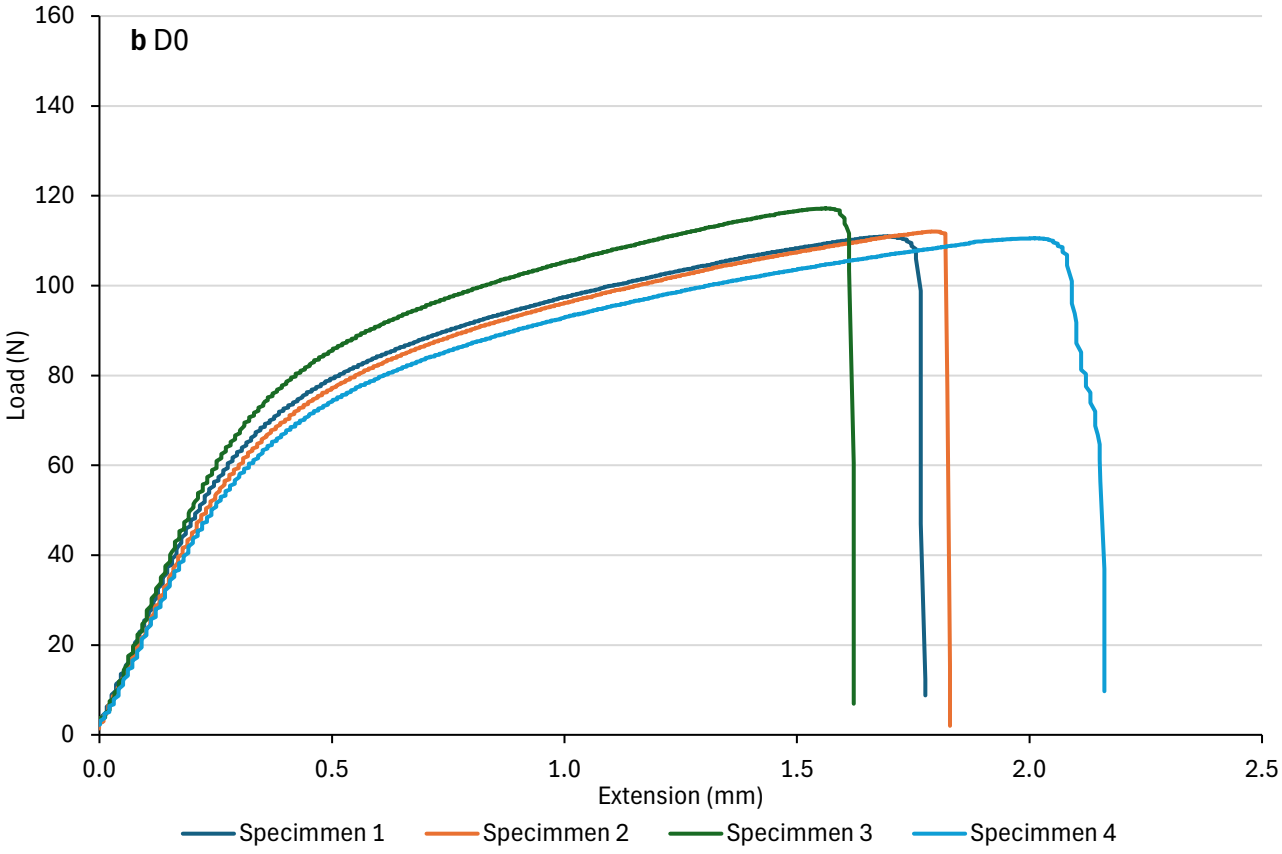
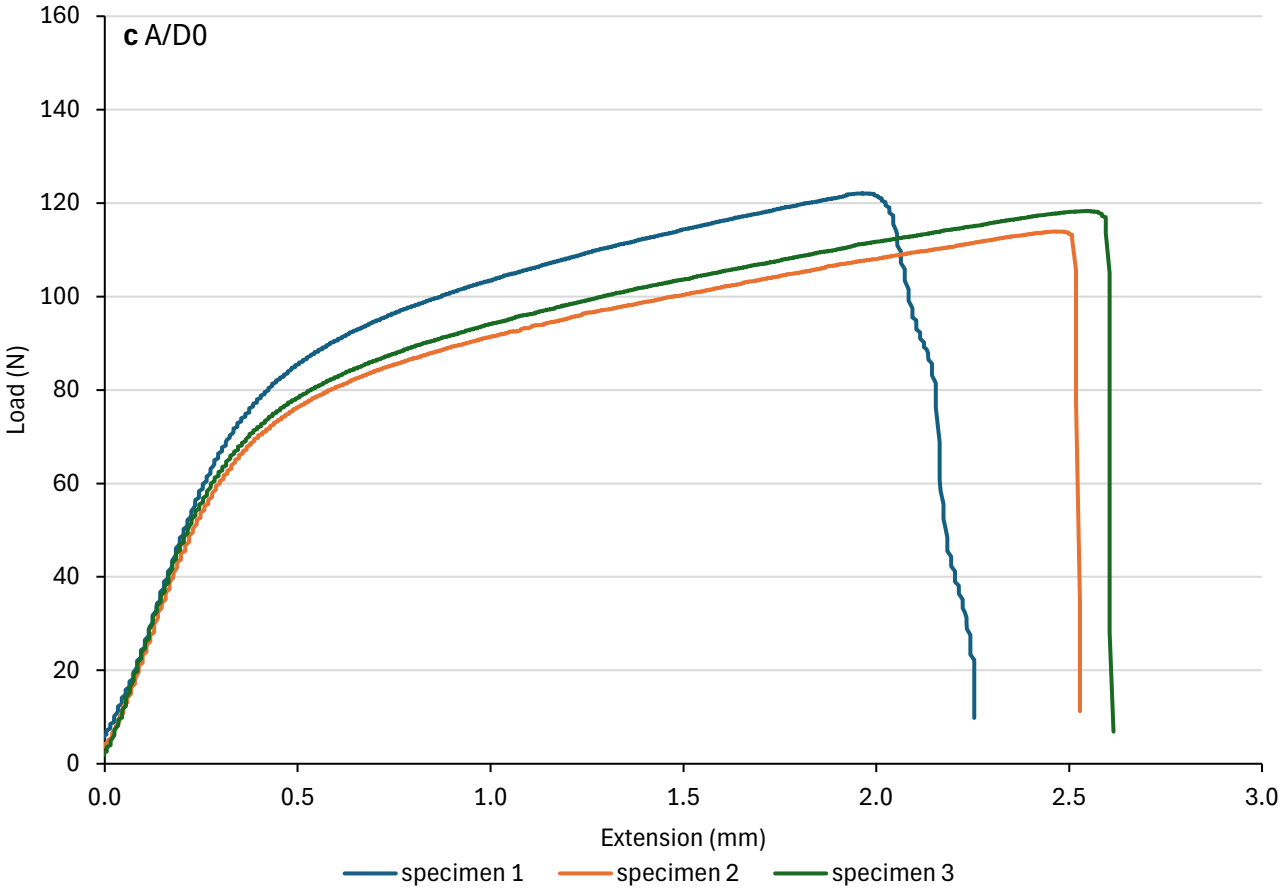
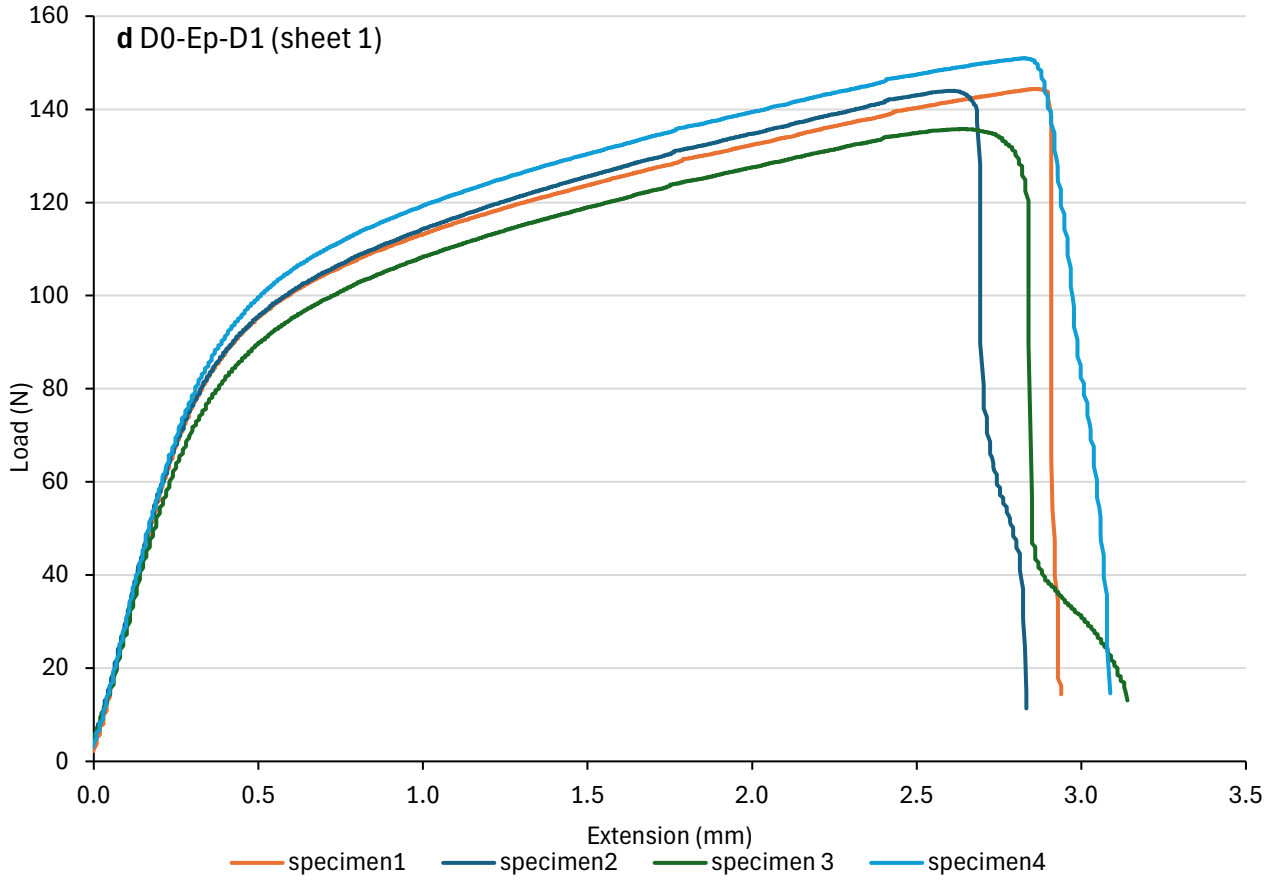


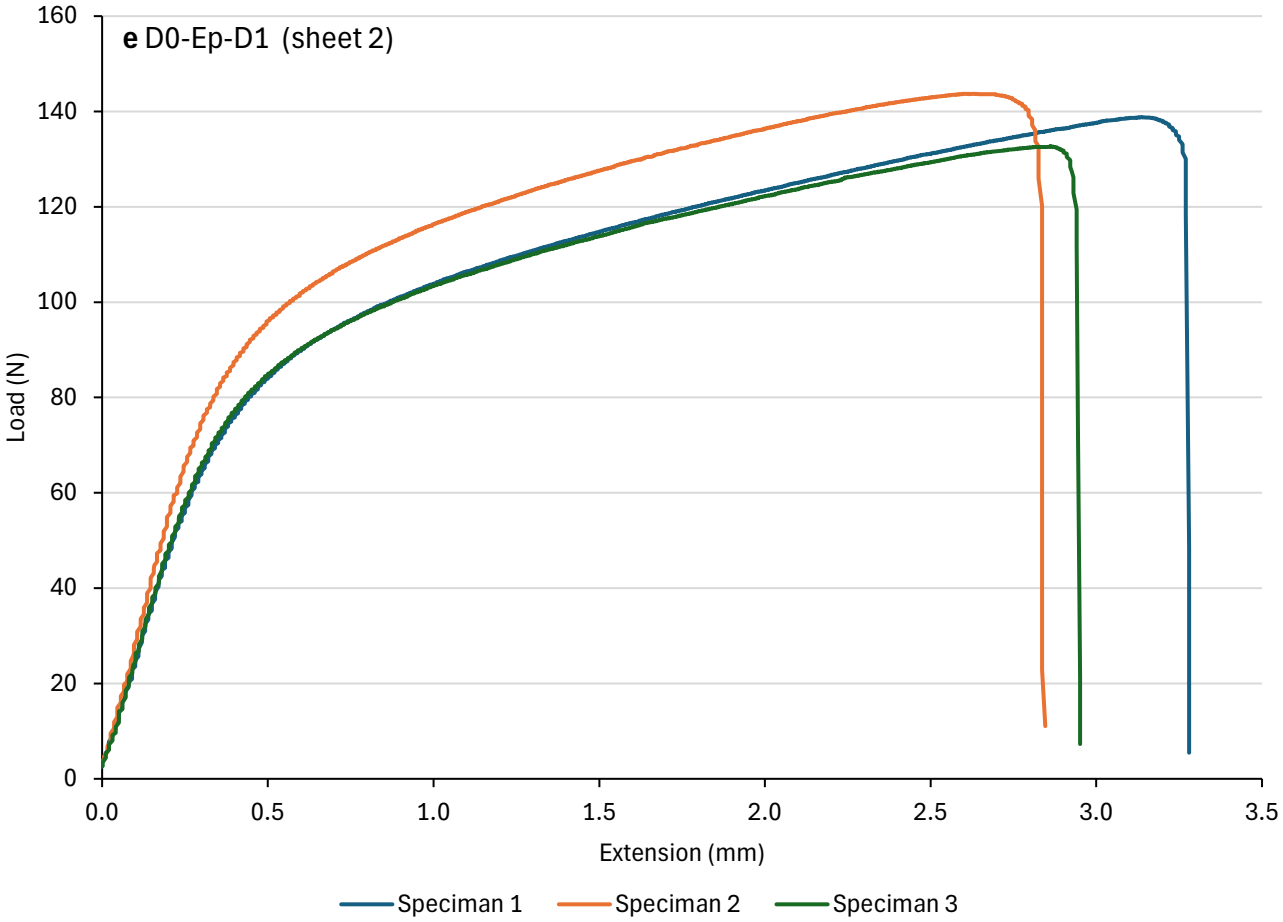
Fig. S13 Tensile properties showing the effect of A-stage in reference to B-P1-P2-C: **a** D0 in comparison to A/D0; D0EpD1 in comparison to A/D0EpD1. Their exact data points and profile properties, as well as their breakage fracture of the pulp sheet, are shown at **Table S6** and **Fig. S12**. **b** Correlation between the loss of viscosity and reduction of tensile index from two series of sample: D0-> A/D0 and D0-Ep-D1-> A/D0-Ep-D1.

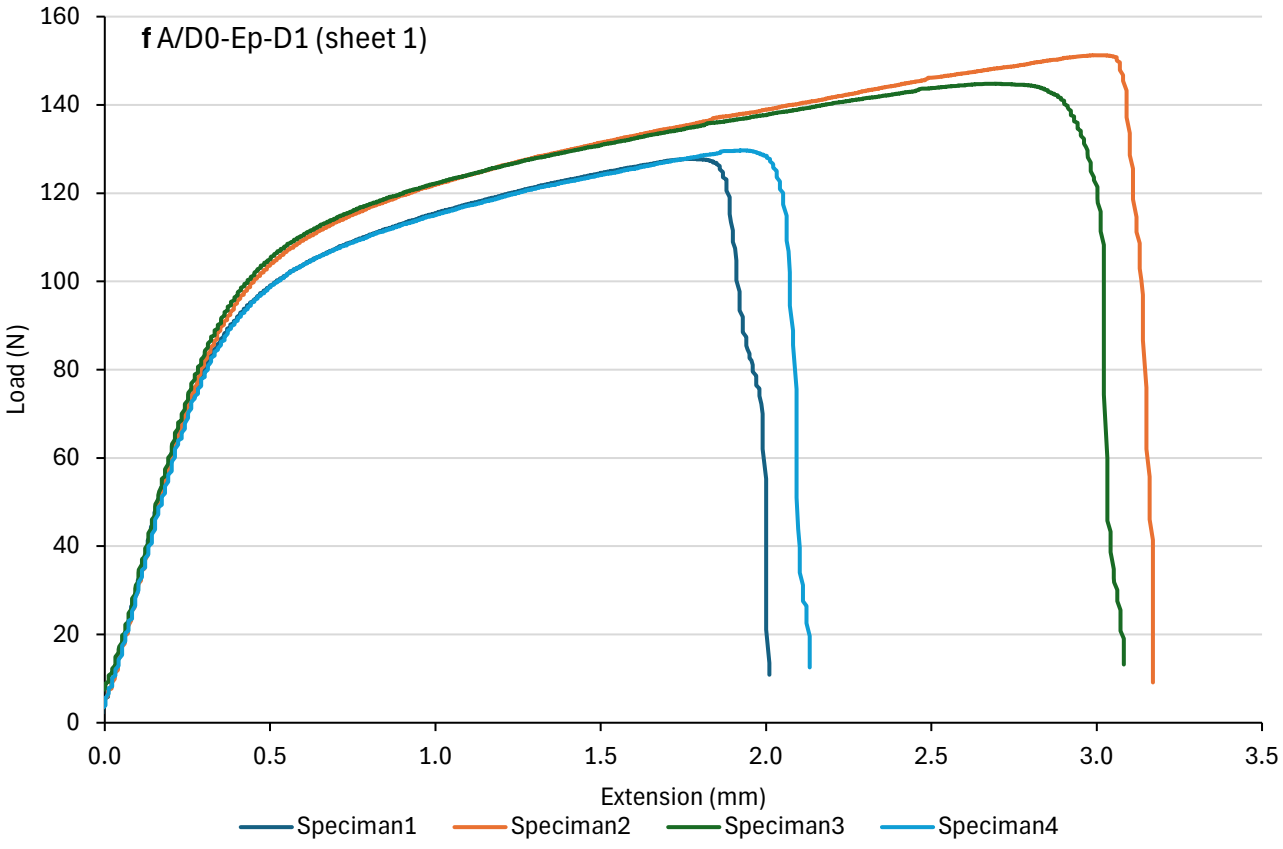

a B-P1-P2-C
160
140
120
100
80
60
40
20
0
Load (N)
0.0
0.5
1.0
1.5
2.0
2.5
Extension (mm)
Speciman 1
Speciman 2
Speciman 3
Speciman 4
Speciman 5


b D0
160
140
120
100
80
60
40
20
0
Load (N)
0.0
0.5
1.0
1.5
2.0
2.5
Extension (mm)
Specimmen 1
Specimmen 2
Specimmen 3
Specimmen 4


c A/D0
160
140
120
100
80
60
40
20
0
Load (N)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Extension (mm)
specimen 1
specimen 2
specimen 3


d D0-Ep-D1 (sheet 1)
160
140
120
100
80
60
40
20
0
Load (N)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Extension (mm)
specimen1
specimen2
specimen 3
specimen4


e D0-Ep-D1 (sheet 2)
160
140
120
100
80
60
40
20
0
Load (N)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Extension (mm)
Speciman 1
Speciman 2
Speciman 3


f A/D0-Ep-D1 (sheet 1)
160
140
120
100
80
60
40
20
0
Load (N)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Extension (mm)
Speciman1
Speciman2
Speciman3
Speciman4

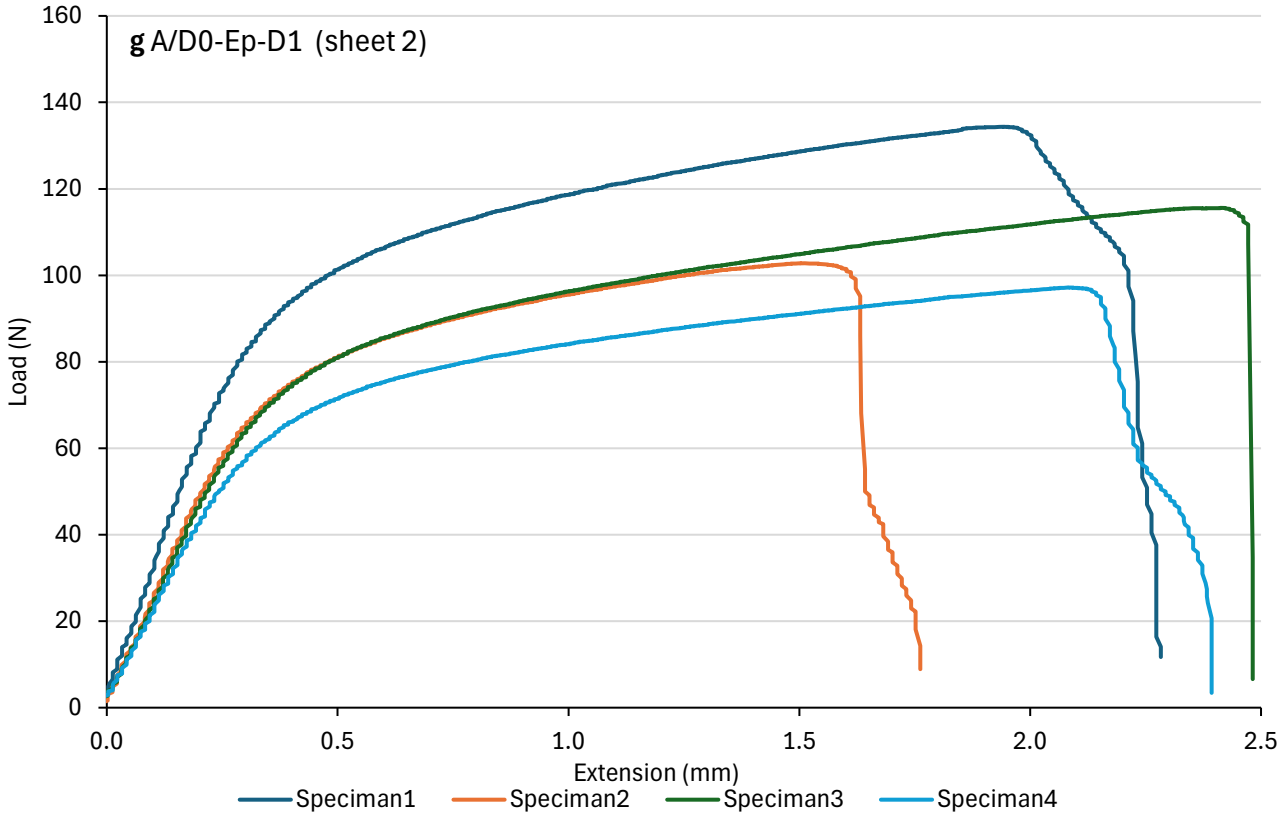


Fig. S14 Load-Extension Curve showing the effect of A-stage in reference to B-P1-P2-C (**a**): **b** D0; **c** A/D0; **d and e** D0EpD1; **f and g** A/D0EpD1. **Fig. S12** visualizes photographs of their fracture surface after the tensile test.

Table S7 Characteristics of the different lignin sources derived from the ultrafiltration (i.e. spent liquor; permeate; and retentate)

		Spent liquor (feed)	Permeate	Retentate
Molecular weight, g/mol	*Mn*	641	487	980
	Mw	2776	839.5	4032
	Mz	8525	1395	9851
	PD	4.3	1.7	4.1
Other characteristics	Density	1.03	0.96	0.98
	pH	11.44	11.11	10.5
	Residual alkali, g NaOH/L	1.97	< 0.5	< 0.5

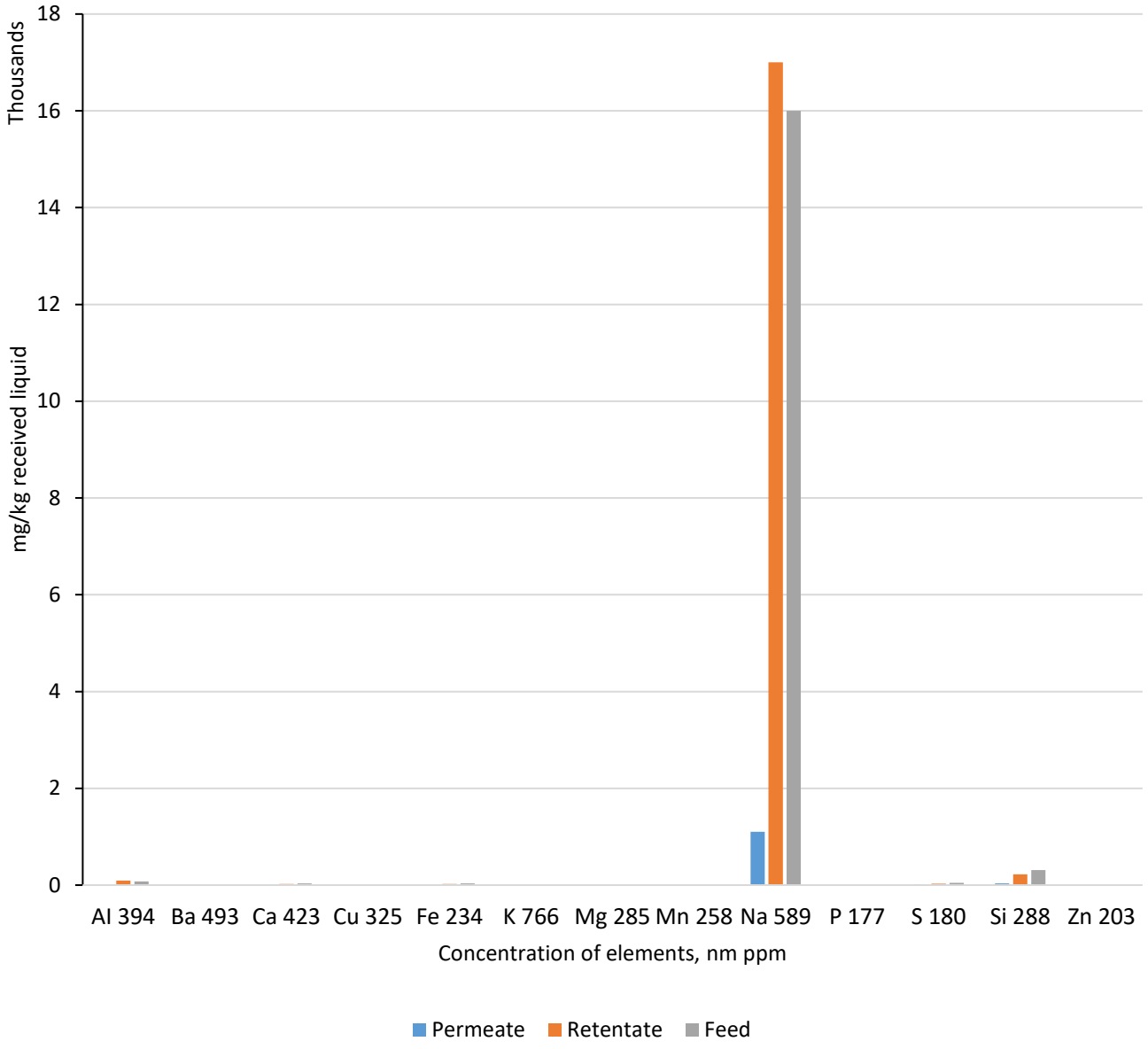


Fig. S15 ICP-OES results of the ultrafiltration related liquids: feed; permeate; retentate.

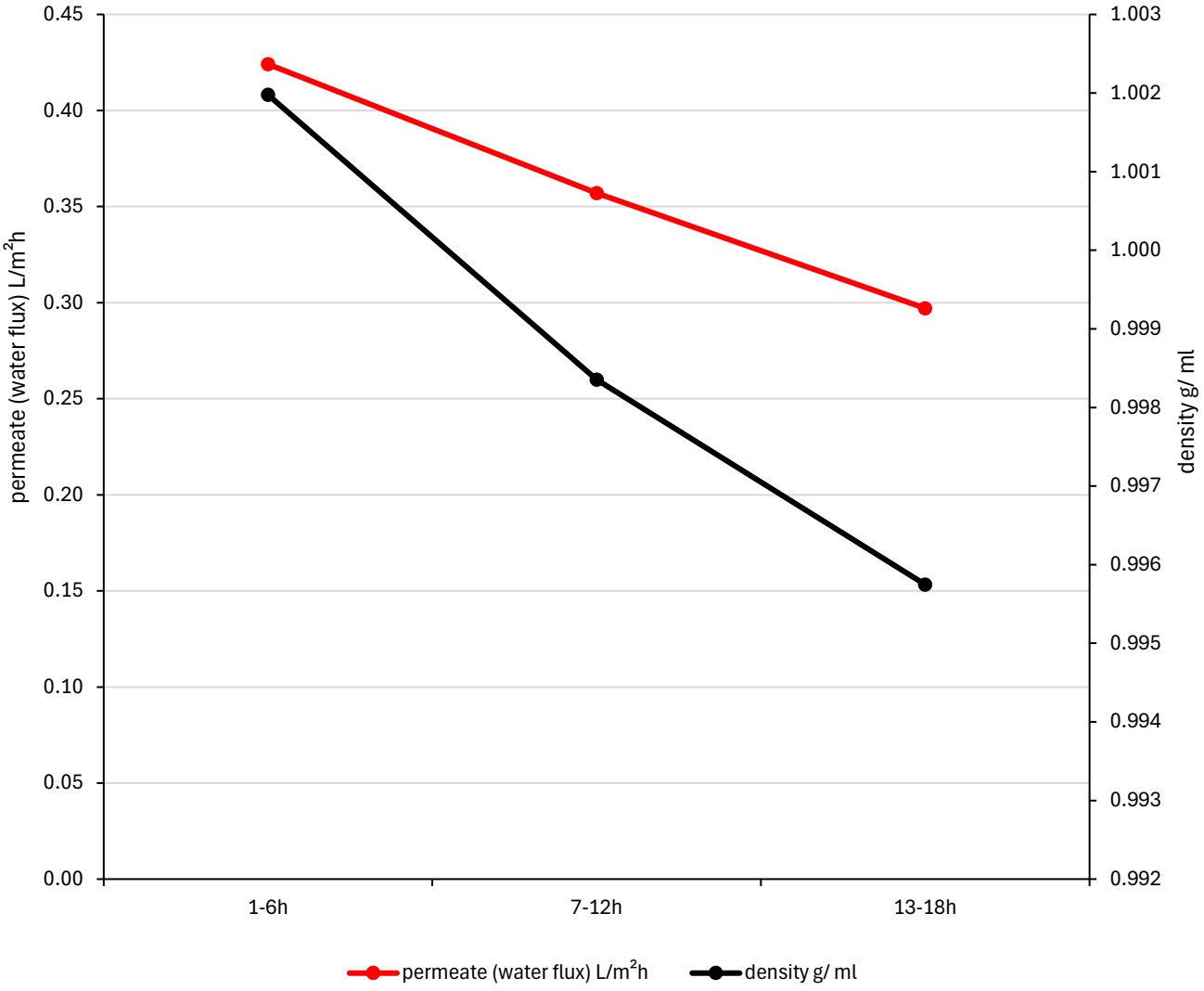
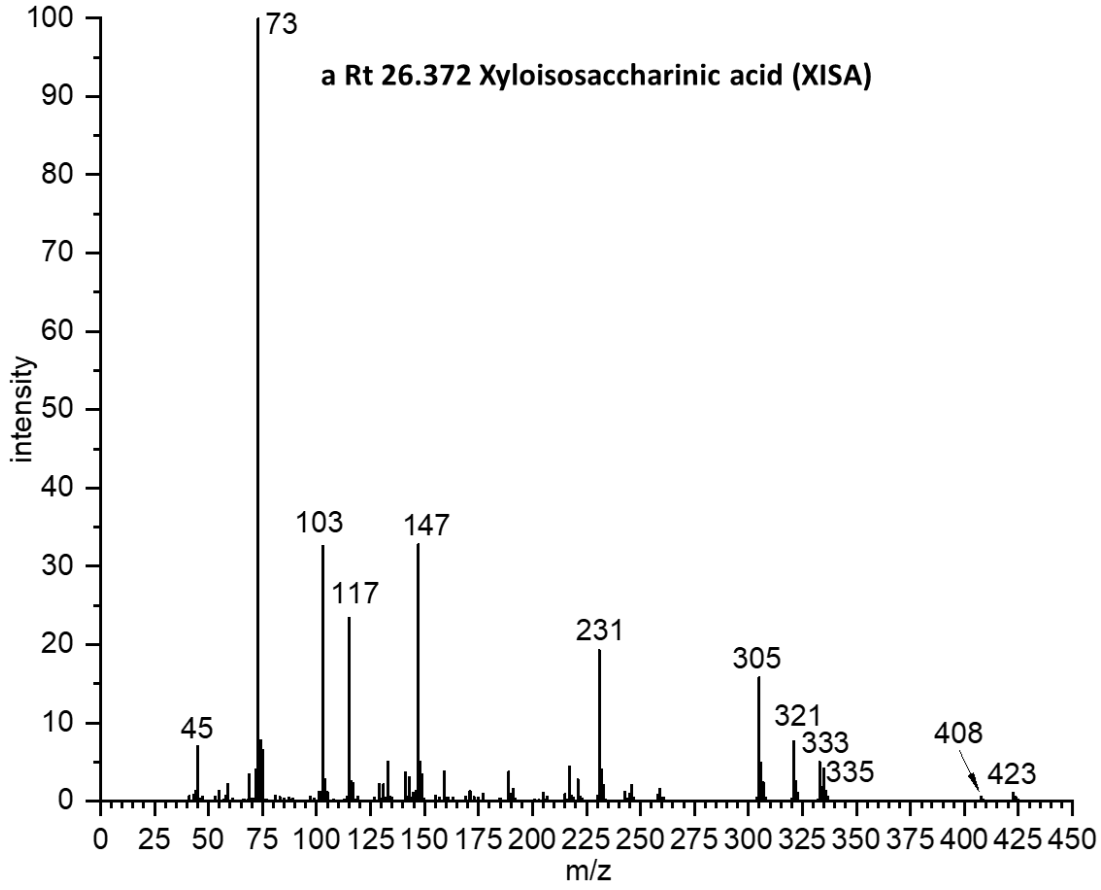
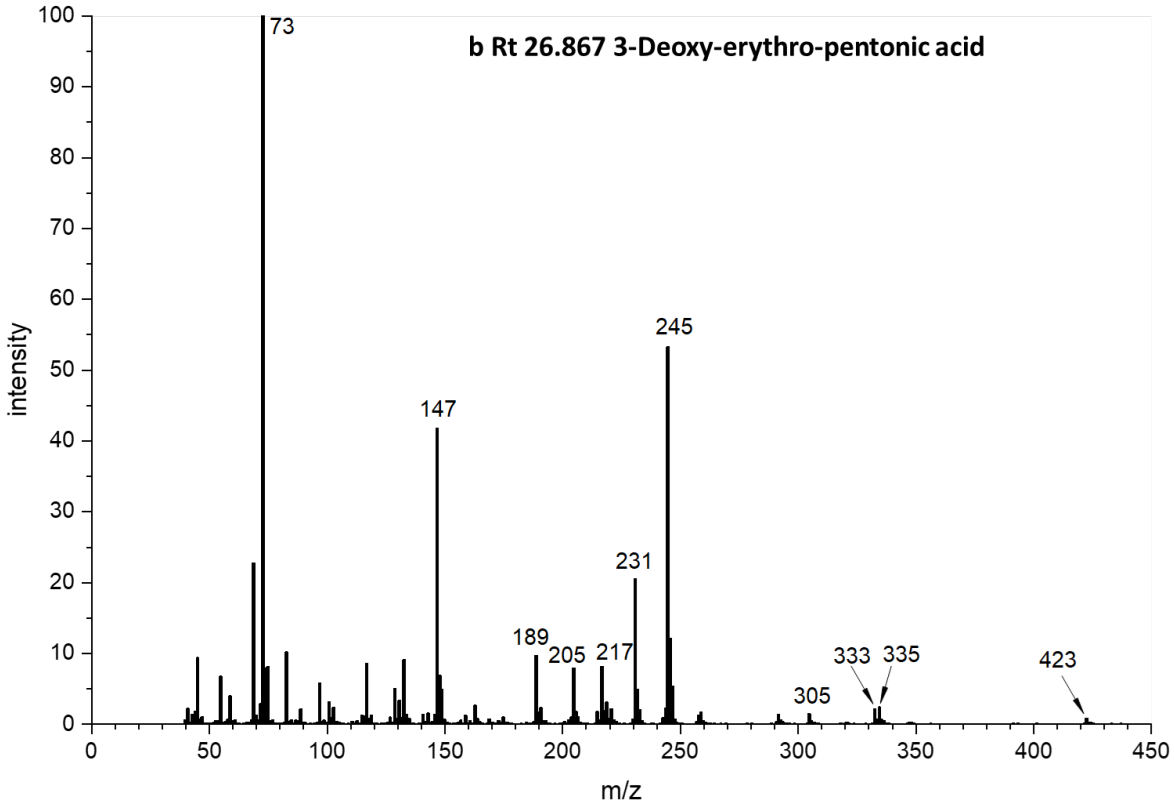
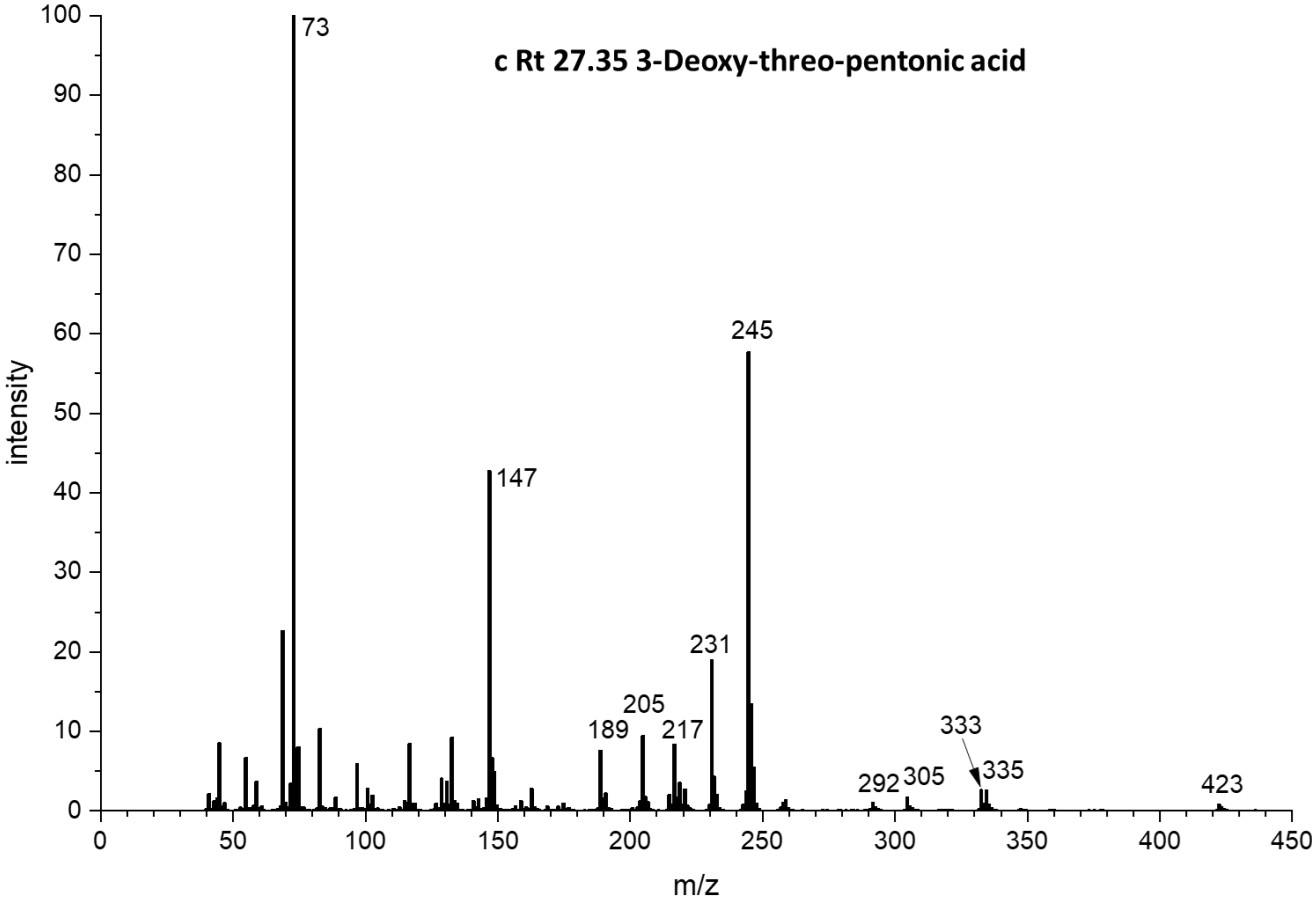
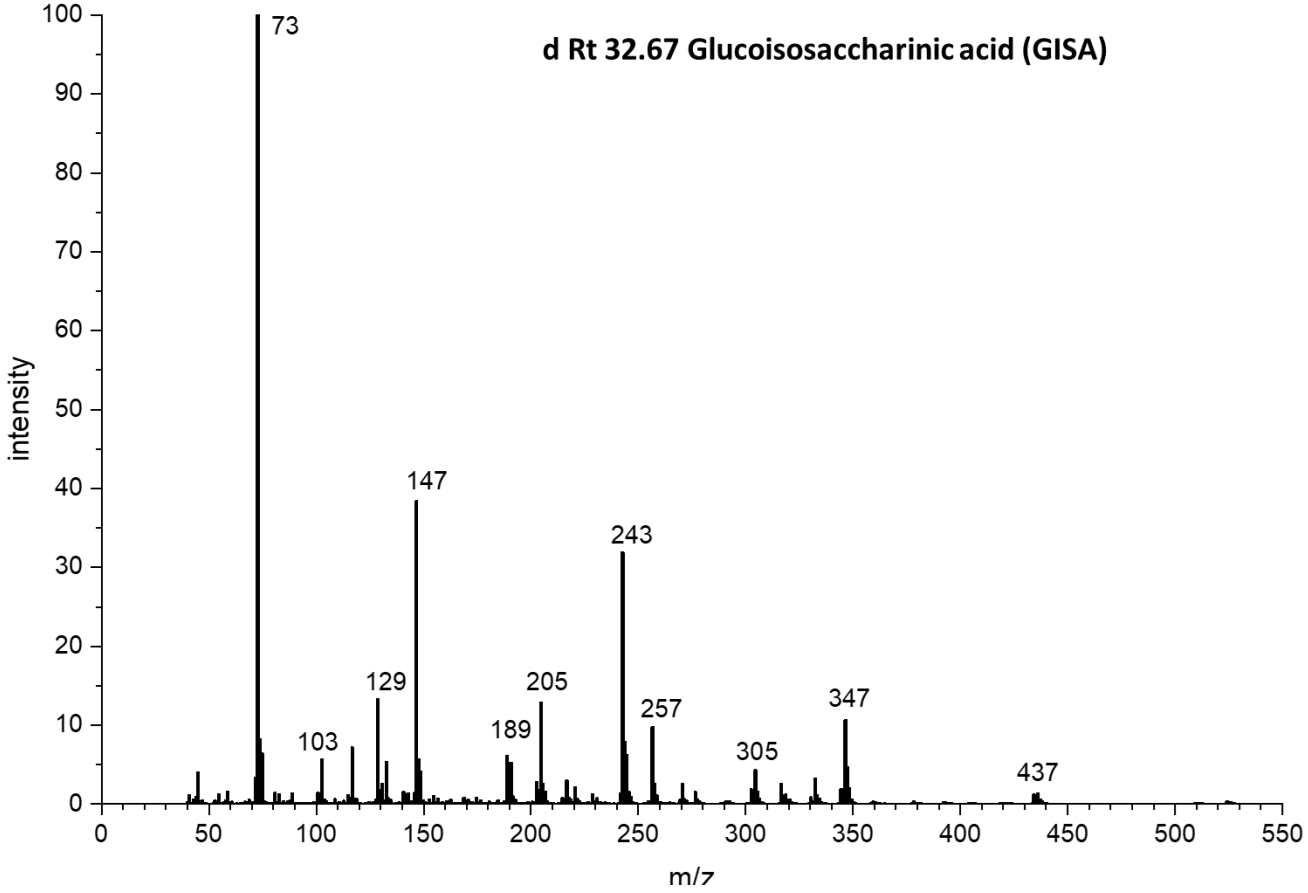


Fig. S16 Trendline of the permeate and density along with three cycles (6 hours/ cycle) of sample collection: 1-6h; 7-12h; 13-18h.


a Rt 26.372 Xyloisosaccharinic acid (XISA)
intensity
m/z
73
103
147
117
231
305
321
333
335
408
423
45


b Rt 26.867 3-Deoxy-erythro-pentonic acid
intensity
m/z
73
245
147
231
189
205
217
333
335
305
423


c Rt 27.35 3-Deoxy-threo-pentonic acid
intensity
m/z
73
147
189
205
217
231
245
292
305
333
335
423


d Rt 32.67 Glucoisosaccharinic acid (GISA)
intensity
m/z
73
103
129
147
189
205
243
257
305
347
437

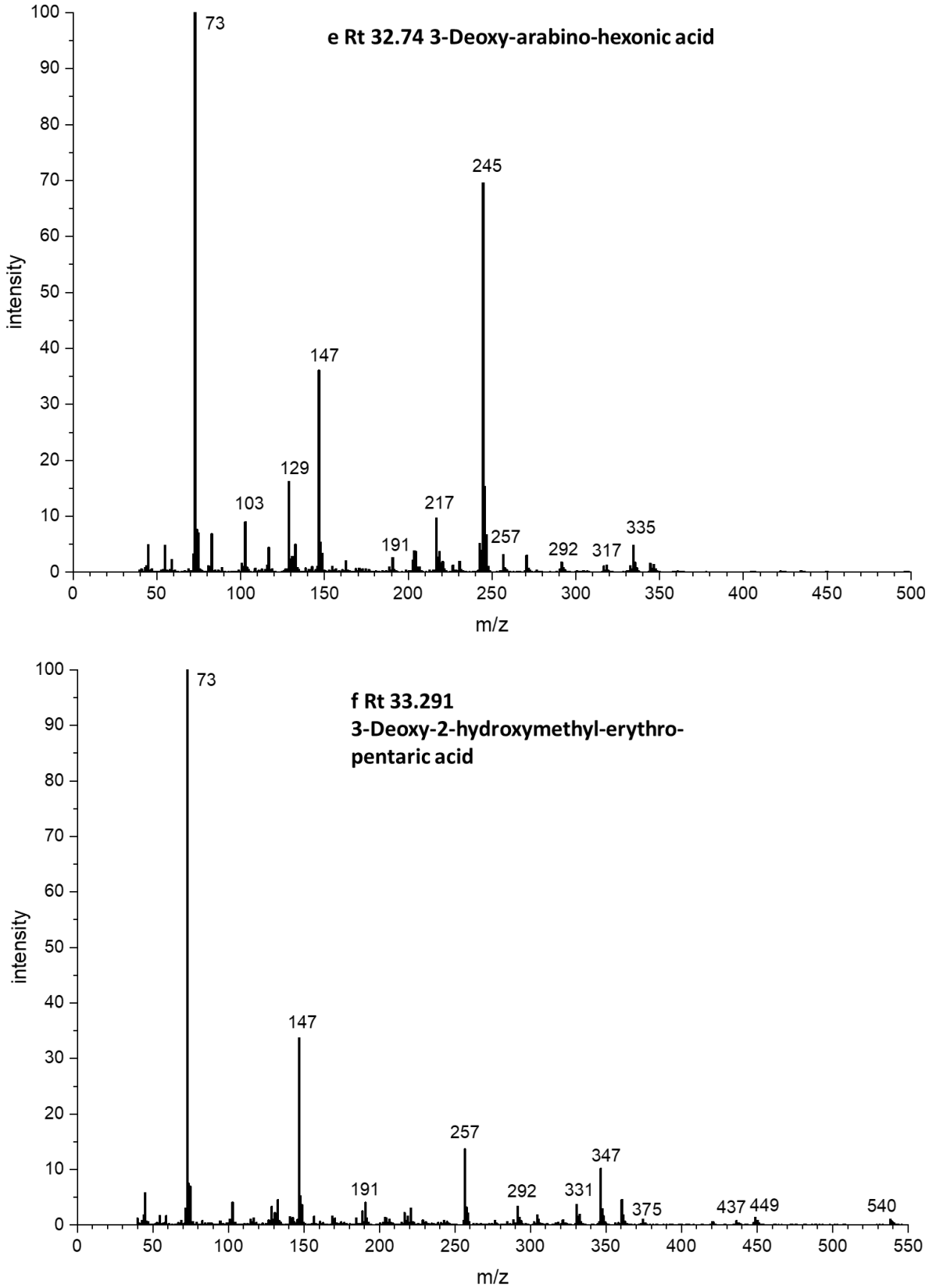


Fig. S17 Mass spectrum of the TMS derivatives of some typical hydroxy acids collected from the spent liquor: **a** Rt 26.372 Xyloisosaccharinic acid (XISA); **b** Rt 26.867 3-Deoxy-erythro-pentonic acid; **c** Rt 27.35 3-Deoxy-threo-pentonic acid; **d** Rt 32.67 Glucoisosaccharinic acid (GISA); **e** Rt 32.74 3-Deoxy-arabino-hexonic acid; **f** Rt 33.291 3-Deoxy-2-hydroxymethyl-erythro-pentaric acid.

Table S8 The quantitative profile (g/L) of the ultrafiltration-related: 1) Feed and 2) Permeate and 3) Retentate after the cut-off 0.5kDa.

code	Ret. Time/	Compound (TMS derivatized form)	Feed	Permeate	Retentate	MW	Characteristic fragments m/z	References and databases
1	7.167	Lactic acid (TMS ester, TMS ether)	0.28	0.18	0.03	234	219; 191; 147; 117; 73	[N]
2	7.251	α-Hydroxyisobutyric acid (TMS ester, TMS ether)	0.01	0.01		248	233; 205; 147; 131	[N]
3	7.633	Glycolic acid (TMS ester, TMS ether)	0.15	0.11	0.02	220	205; 177; 147; 73	[N]
4	9.482	2-Hydroxybutanoic acid (2-HBA) (TMS ester, TMS ether)	0.25	0.17	0.03	248	233; 205; 147; 131; 73	[N]
5	9.676	Oxalic acid (di TMS ester)	0.04	0.02	0.003	234	219; 190; 147; 73	[N]
6	10.006	Hydracrylic acid (TMS ester, TMS ether)	0.004	0.0027		234	219; 177; 147; 73	[N]
7	11.313	Orthosilicic acid (tetra TMS ether)	0.001	0.001		384	369; 281; 147; 73	[N]
8	13.255	4-Hydroxybutanoic acid (TMS ester, TMS ether)	0.012	0.01		248	233; 147; 117; 73	[N]
9	13.421	Benzoic Acid (TMS ester)		0.0015		194	194; 179; 135; 105; 77	[N]
10	14.898	Glycerol (tri TMS ether)	0.014	0.02		308	293; 218; 205; 147; 73	[N]
11	15.965	Succinic acid (di TMS ester)	0.013	0.01		262	262; 247; 147; 133; 129; 75; 73	[N]
12	16.402	Methylsuccinic acid (di TMS ester)	0.004	0.002		276	261; 232; 217; 147; 129; 73	[N]
13	16.402	2,3-Dihydroxy-2-methylpropanoic acid (TMS ester, di TMS ether)	0.004	0.002		336	336; 321; 306; 233; 219; 147	[N]
14	16.734	2-Hydroxyhexanoic acid (TMS ester, TMS ether)	0.002	0.001		276	261; 233; 159; 147; 73	[N]
15	16.835	Glyceric acid (TMS ester, di TMS ether)	0.004	0.0035		322	307; 292; 205; 189; 147; 133; 103; 73	[N]
16	17.643	4-Hydroxybenzaldehyde (TMS ether)	0.009	0.01		194	194; 179; 151	[N]
17	18.890	Tartronic acid (TMS ether, di TMS ester)	0.011	0.001		336	321; 292; 221; 147; 133; 102; 73	[N]; [A]
18	19.529	2,4-Dihydroxybutanoic acid (TMS ester, di TMS ether)	0.021	0.02	0.001	336	321; 219; 203; 147; 129; 103; 73	[N]
19	21.225	4-(2-amino-1-hydroxyethyl)phenol (di TMS ether)	0.012	0.01		297	282; 267; 193; 73	[N]
20	21.956	Malic acid (di TMS ester, TMS ether)	0.012	0.01		350	335; 307; 245; 233; 147; 73	[N]
21	22.526	2,5- Dihydroxy pentanoic acid (2,5-DHPA) (TMS ester, di TMS ether)	0.096	0.08	0.01	350	335; 233; 217; 147; 143; 73	17
22	22.880	Vanillin (TMS ether)	0.004	0.0029		224	224; 209; 194; 73	[N]
23	24.514	2-Hydroxyglutaric acid (TMS ether, di TMS ester)	0.012	0.005		364	349; 247; 203; 147; 133; 129; 73	[N]

24	24.587	2-Hydroxy-2-methylpentanedioic acid (di TMS ester, TMS ether)	0.001492	0.001		378	363; 335; 261; 147; 143	[N]
25	26.372	Xyloisosaccharinic acid (XISA) (tri TMS ether; TMS ester)	0.105	0.08	0.01	438	423; 408; 333; 321; 305	9
26	26.867	3-Deoxy-erythro-pentonic acid (TMS ester, tri TMS ether)	0.015	0.01	0.002	438	423; 335; 305; 245; 205; 147; 133; 73	17;18
27	27.252	2-Hydroxyadipic acid (di TMS ester, TMS ether)	0.005	0.002		378	363; 335; 261; 245; 203; 171; 147; 129; 73	[N]
28	27.353	3-Deoxy-threo-pentonic acid (TMS ester, tri TMS ether)	0.049	0.04	0.004	438	423; 335; 305; 245; 205; 147; 133; 73	17;18
29	27.701	Syringaldehyde (TMS ether)	0.002	0.002		254	254; 239; 224	[N]
30	28.238	Levoglucosan (tri TMS ether)	0.002	0.001		378	333; 217; 204; 147; 117; 103; 73	[N]
31	29.467	Vanillic acid (TMS ether, TMS ester)	0.003	0.001		312	312; 297; 282; 267; 253; 223; 193; 165; 133; 126; 73	[N]
32	32.665	Glucoisosaccharinic acid (GISA) (tetra TMS ether, TMS ester)	0.134	0.10	0.01	540	525; 435; 347; 243; 205; 147; 129; 73	17; 19
33	32.706	3-Deoxy-arabino-hexonic acid (TMS ester, tetra TMS ether)	0.025	0.02		540	525; 335; 245; 217; 147; 129	17; 19
32	32.940	Glucoisosaccharinic acid (GISA) (tetra TMS ether, TMS ester)	0.061	0.05	0.005	540	525; 435; 347; 243; 205; 147; 129; 73	17; 19
34	32.998	Syringic acid (TMS ester, TMS ether)	0.002	0.0027		342	342; 327; 312; 297; 283; 253; 223	[N]
35	33.291	3-Deoxy-2-hydroxymethyl-erythro-pentaric acid (di TMS ester, tri TMS ether)	0.006	0.0030		555	540; 449; 437; 375; 347; 331; 292; 257	17; 19
36	33.803	4-Coumaric acid (TMS ester, TMS ether)	0.005	0.002		308	308; 293; 249; 219; 73	[N]
37	33.858	3-Deoxy-2-hydroxymethyl-threo-pentaric acid (di TMS ester, tri TMS ether)	0.002	0.002		555	540; 449; 437; 375; 347; 331; 292; 257	17; 19
38	37.462	Ferulic acid (TMS ester, TMS ether)	0.003	0.001		338	338; 323; 308; 249; 219; 73	[N]
39	52.641	9,10,18-Trihydroxystearic acid (TMS ester, tri TMS ether)	0.002	0.001		620	605; 515; 390; 317; 303; 217; 147; 129; 73	[N]