

Oxidation of flame retardant tetrabromobisphenol A by a biocatalytic nanofiber of chloroperoxidase

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Table S1. Partial physicochemical characterization of environmental water samples.

Parameter	Groundwater	Surface water ¹			Treated wastewater ²	
		Lagoon	River A	River B	WWTP A	WWTP B
pH	6.55	8.84	7.42	7.54	7.52	7.27
BOD (mg O ₂ /L)	2.0	3.0	20.0	5.5	160.0	37.0
COD (mg O ₂ /L)	5.0	8.5	832.0	16.5	781.5	104.0
TDS (m/L)	652.0	452.0	681.0	636.0	1120.0	1349.0
Conductivity (μS/cm)	921.0	593.0	1313.0	872.0	2260.0	1423.0
Free Chloride (mg/L)	0.09	0.05	0.0	0.165	0.14	0.05
NO ₃ ¹⁻ (mg/L)	4.05	27.45	0.0	39.70	80.0	268.00
PO ₄ ³⁻ (mg/L)	0.68	1.78	3.5	0.51	45.0	106.50
SO ₄ ²⁻ (mg/L)	96.0	74.0	175.0	137.0	95.0	97.0
Mg ²⁺ (mg/L)	10.0	15.0	35.0	20.0	65.0	15.0
Ca ²⁺ (mg/L)	0.0	103.5	160.0	10.0	200.0	0.0
Fe ³⁺ (μg/L)	66.0	18.0	0.375	36.0	1310.0	--

¹ River A: Nexapa River and River B: Chapa-Chapa River; ²WWTP A: from Puebla State and WWTP B: from Puebla city.

Table S2. FTIR characterization of nanofibers and their precursors.

Characteristic group	Wavenumber (cm ⁻¹)		
	Chitosan	PVA	Nanofibers
v(NH ₂) assoc. in primary amines and v(OH) asoc. in pyranose ring	3362	–	3348
v(OH) from intermolecular and intramolecular hydrogens bonds	–	3335	3348
v(CH ₂) in alkyl groups	–	2938	2938
v(C-H) in pyranose ring and alkyl groups	2875	2915	2916
v(C=O) as polyvinyl acetate residual	–	1734	1747
v(C=O) as polyvinyl acetate residual	–	1722	1722
v(NH ₂) in NHCOCH ₃ group (Amide I band)	1652	–	1665
v(NH) in NHCOCH ₃ group (Amide II band)	1593	–	1582
δ(CH ₂) in CH ₂ OH group	1418	1429	1429
δ _s (CH ₃) in NHCOCH ₃ and methyl groups	1374	1374	1377
δ(C-H) in carbon chain	1316	1326	1324
v(CO-O-C) as polyvinyl acetate residual	–	1245	1248
v _s (C-O-C) glycosidic linkage	1151	–	1147
v(C-O) in C-OH groups	–	1088	1083
v _{as} (C-O-C) glycosidic linkage	1057	–	–
v(C-O) in secondary OH group	1026	1026	1035
CH ₃ CO group in pyranose ring	895	–	905
v(C-C) in carbon chain	–	848	852