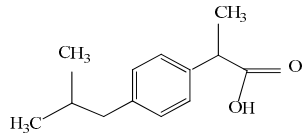
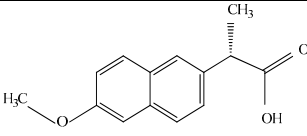
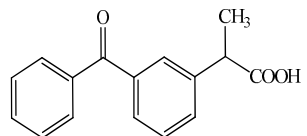
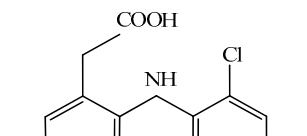
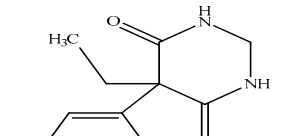
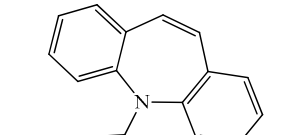
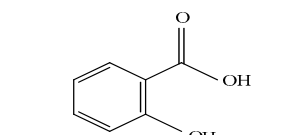
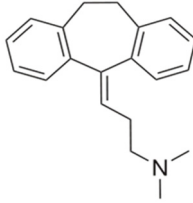
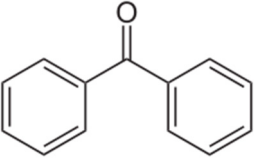
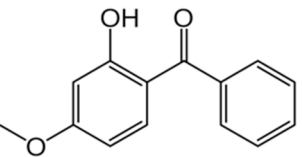
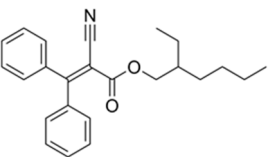


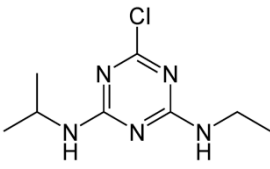
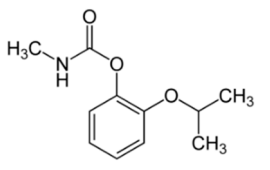
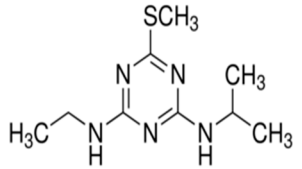
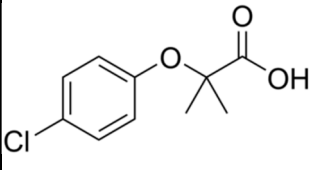
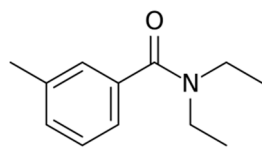
Supplementary Materials: Degradation of Trace Organic Contaminants by a Membrane Distillation—Enzymatic Bioreactor

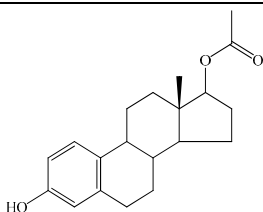
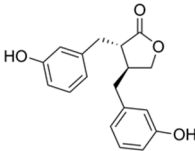
Muhammad B. Asif, Faisal I. Hai, Jinguo Kang, Jason P. van de Merwe, Frederic D.L. Leusch, Kazuo Yamamoto, William E. Price and Long D. Nghiem

Table S1. Physicochemical properties of the selected trace organic contaminants (TrOCs).

Category	Compound (CAS number)	Molecular weight (g/mol)	Log K _{OW} ^a	Log D (pH 7) ^a	Dissociation constant (pK _a) ^a	Limit of detection (ng/L) ^b	Chemical structure
Pharmaceuticals	Ibuprofen (C ₁₃ H ₁₈ O ₂) (5687-27-1)	206.28	3.50 ± 0.23	0.94	4.41 ± 0.10	20	
	Naproxen (C ₁₄ H ₁₄ O ₃) (22204-53-1)	230.26	2.88 ± 0.24	0.73	4.84 ± 0.30	1	
	Ketoprofen (C ₁₆ H ₁₄ O ₃) (22071-15-4)	254.28	2.91 ± 0.33	0.19	4.23 ± 0.10	20	
	Diclofenac (C ₁₄ H ₁₁ Cl ₂ NO ₂) (15307-86-5)	296.15	4.55 ± 0.57	1.77	4.18 ± 0.10 -2.26 ± 0.50	5	
	Primidone (C ₁₂ H ₁₄ N ₂ O ₂) (125-33-7)	218.25	0.83 ± 0.50	0.83	12.26 ± 0.40 -1.07 ± 0.40	10	
	Carbamazepine (C ₁₅ H ₁₂ N ₂ O) (298-46-4)	236.27	1.89 ± 0.59	1.89	13.94 ± 0.20 -0.49 ± 0.20	10	
	Salicylic acid (C ₇ H ₆ O ₃) (69-72-7)	138.12	2.01 ± 0.25	-1.13	3.01 ± 0.10	1	

	Metronidazole (C ₆ H ₉ N ₃ O ₃) (443-48-1)	171.15	-0.14 ± 0.30	-0.14	14.44 ± 0.10 2.58 ± 0.34	20	
	Gemfibrozil (C ₁₅ H ₂₂ O ₃) (25812-30-0)	250.33	4.30 ± 0.32	2.07	4.75	1	
	Amitriptyline C ₂₀ H ₂₃ N (50-48-6)	277.40	4.40±0.2 6	2.28	9.18±0.28	1	
Personal care products	Triclosan (C ₁₂ H ₇ Cl ₃ O ₂) (3380-34-5)	289.54	5.34 ± 0.79	5.28	7.80 ± 0.35	1	
	Benzophenone C ₁₃ H ₁₀ O (119-61-9)	182.22	3.21 ± 0.29	3.21	-	5	
	Oxybenzone C ₁₄ H ₁₂ O ₃ (131-57-7)	228.24	3.99±0.3 6	3.89	7.56±0.35	5	
	Octocrylene C ₂₄ H ₂₇ N O ₂ (6197-30-4)	361.48	6.89±0.3 3	6.89	-	10	
Pesticides	Fenoprop (C ₉ H ₇ Cl ₃ O ₃) (93-72-1)	269.51	3.45 ± 0.37	-0.13	2.93	20	

	Pentachloro-phenol (C ₆ HCl ₅ O) (87-86-5)	266.34	5.12 ± 0.36	2.85	4.68 ± 0.33	1	
	Atrazine (C ₈ H ₁₄ ClN ₅) (1912-24-9)	215.68	2.636±0.205	2.64	2.27±0.10	10	
	Propoxur (C ₁₁ H ₁₅ NO ₃) (114-26-1)	209.24	1.538±0.229	1.54	12.28±0.46 -1.49±0.70	1	
	Ametryn (C ₉ H ₁₇ N ₅ S) (843-12-8)	227.33	2.967±0.12	2.97	3.71±0.41	10	
	Clofibric acid (C ₁₀ H ₁₁ ClO ₃) (882-09-7)	214.65	2.425±0.273	-1.06	3.18 ±0.10	1	
	DEET (C ₁₂ H ₁₇ NO) (134-62-3)	191.27	2.42 ± 0.23	2.42	-1.37 ± 0.7	1	
Industrial chemicals	4-tert-butylphenol (C ₁₀ H ₁₄ O) (98-54-4)	150.22	3.39 ± 0.21	3.40	10.13 ± 0.13	1	
	4-tert-octylphenol (C ₁₄ H ₂₂ O) (140-66-9)	206.32	5.18 ± 0.20	5.18	10.15 ± 0.15	1	

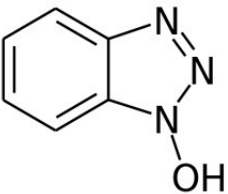
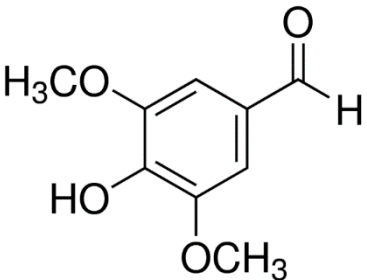
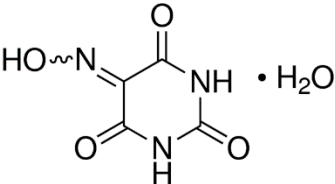
	Bisphenol A (C ₁₅ H ₁₆ O ₂) (80-05-7)	228.29	3.64 ± 0.23	3.64	10.29 ± 0.10	1	
Steroid hormones	Estrone (C ₁₈ H ₂₂ O ₂) (53-16-7)	270.37	3.62 ± 0.37	3.62	10.25 ± 0.40	5	
	17β-estradiol (C ₁₈ H ₂₄ O ₂) (50-28-2)	272.38	4.15 ± 0.26	4.15	10.27	5	
	17β-estradiol 17- acetate (C ₂₀ H ₂₆ O ₃) (1743-60-8)	314.42	5.11 ± 0.28	5.11	10.26 ± 0.60	5	
	17α - ethinylestradiol (C ₂₀ H ₂₄ O ₂) (57-63-6)	269.40	4.10 ± 0.31	4.11	10.24 ± 0.60	10	
	Estriol (E3) (C ₁₈ H ₂₄ O ₃) (50-27-1)	288.38	2.53 ± 0.28	2.53	10.25 ± 0.70	10	
Phytoestrogens	Enterolactone C ₁₈ H ₁₈ O ₄ (78473-71-9)	298.33	1.89± 0.37	1.89	9.93± 0.10	10	

^a Source: SciFinder database <https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf>

Log *D* is logarithm of the distribution coefficient which is the ratio of the sum of concentrations of all forms of the compound (ionised and unionised) in octanol and water at a given pH.

^bLimit of detection (LOD) of the compounds during GC-MS analysis as described in Section 2.5.2. LOD is defined as the concentration of an analyte giving a signal to noise (S/N) ratio greater than 3. The limit of reporting was determined using an S/N ratio of greater than 10.

Table S2. Physicochemical properties of the selected redox-mediators.

Redox mediator	Type	Free radical generated	Oxidation mechanism	Natural/synthetic	Chemical structure
1-hydroxybenzotriazole (HBT)	N – OH	=N – O* Aminoxyl	HAT	Synthetic	
Syringaldehyde (SA)	C ₆ H ₄ (OH)(OC H ₃)	C ₆ H ₅ O* Phenoxyl	HAT	Natural	
Violuric acid (VA)	N – OH	=N – O* Aminoxyl	HAT	Natural	

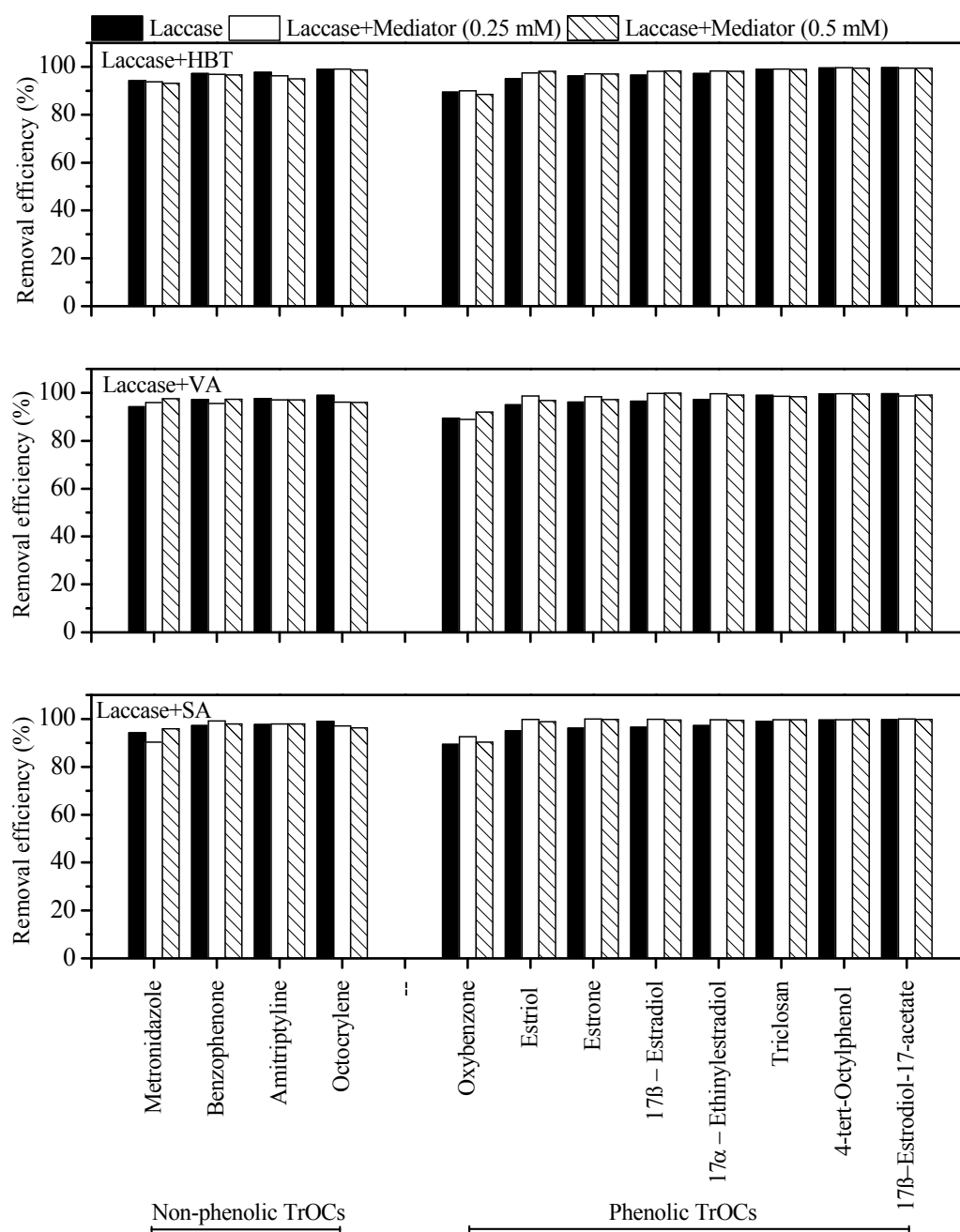


Figure S3. Impact of mediator concentration (0.25 and 0.5 mM) on the degradation of after an incubation time of 12 h in the MD-EMBR. Error bars indicate the standard deviation of duplicate samples. Degradation of these TrOCs did not improve by increasing mediator concentration.

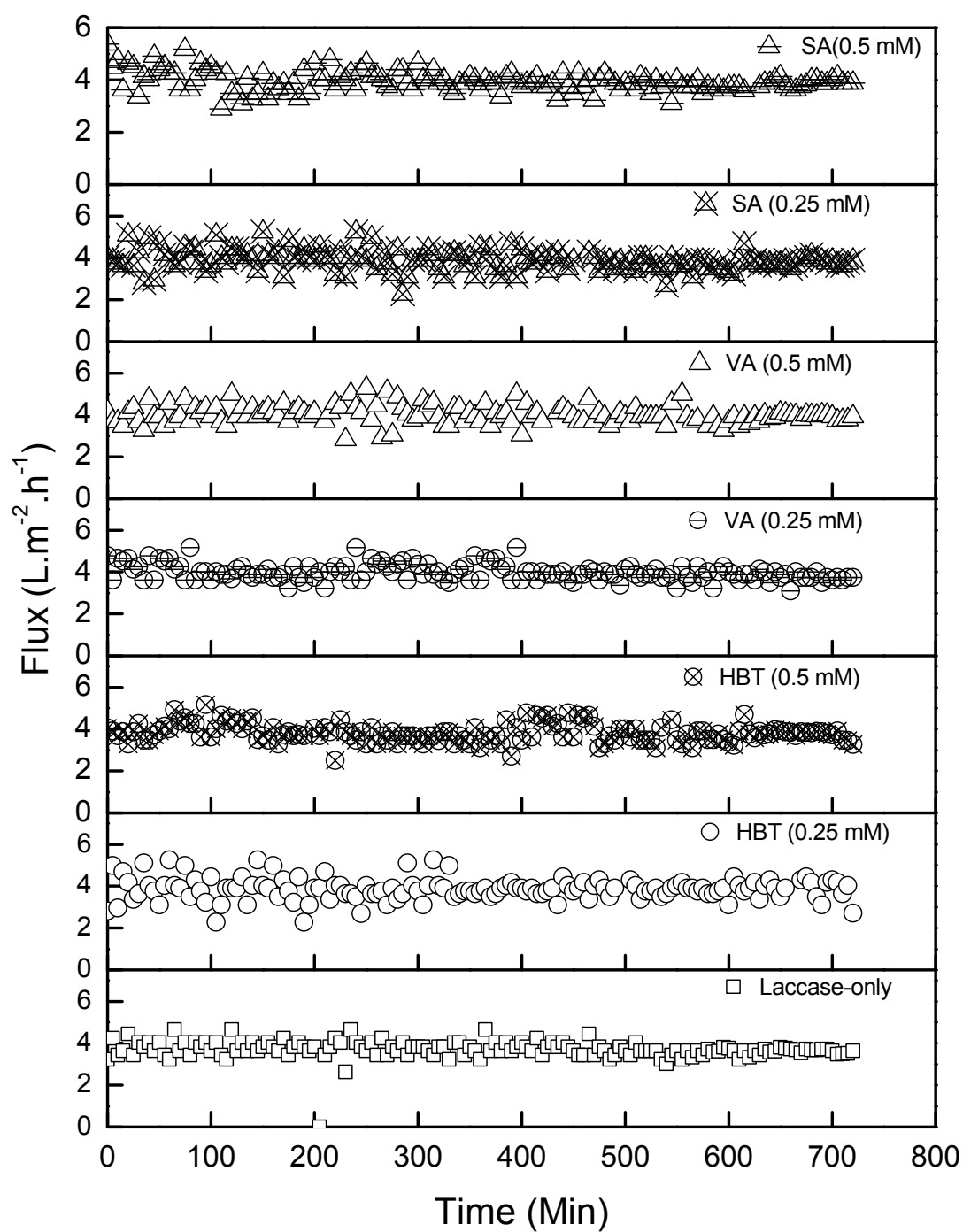


Figure S4. Permeate flux obtained during the operation of enzymatic membrane distillation (MD-EMBR) with and without the addition of redox mediators.