

# **Electrochemical treatment of effluent for the removal of contaminants of emergent concern and culturable microorganisms**

**Joana Dionísio, Cristiana Gonçalves, Paula Guedes, Alexandra B. Ribeiro\*, Nazaré Couto\***

CENSE - Center for Environmental and Sustainability Research, Department of Environmental Sciences and Engineering, NOVA School of Science and Technology, NOVA University Lisbon. 2829-516 Caparica, Portugal

*\*Corresponding authors: abr@fct.unl.pt (A.B.R.); md.couto@fct.unl.pt (N.C.)*

**Table S1.** Physicochemical properties of each contaminant of emergent concern used in this study.

Compound (abbreviation)	CAS	Chemical structure	Molecula r weight (g/mol)	Solubility in water (mg/L)	$K_H$ (atm-cu m/mole)	pKa	Log $K_{ow}$	Log $K_{oc}$
Caffeine (CAF)	58-08-2		194.19	2.16x10 <sup>4</sup> <sup>(a)</sup>	1.1x10 <sup>-11</sup>	0.7/14.0	-0.07	2.87 – 3.89 <sup>(e)</sup>
Carbamazepine (CBZ)	298-46-4		236.27	17,7 <sup>(c)</sup>	1.1x10 <sup>-10</sup>	13.9	2.45	2.71
Oxybenzone (OXY)	131-57-7		228.25	69 <sup>(a)</sup>	1.5x10 <sup>-8</sup>	8.07	3.79	2.98
Diclofenac (DCF)	15307-86-5		296.15	2.37 <sup>(a)</sup>	6.1x10 <sup>-8</sup>	4.15	4.51	2.39
Triclosan (TCS)	3380-34-5		289.54	10 <sup>(b)</sup>	2.1x10 <sup>-8</sup>	7.90	4.76	3.38 – 4.20
Bisphenol A (BPA)	80-05-7		228.29	120 <sup>(c)</sup>	4.0x10 <sup>-11</sup>	9.60	3.32	2.06 – 3.59
17 $\beta$ -estradiol (E2)	50-28-2		272.40	3,6 <sup>(e)</sup>	3.6x10 <sup>-11</sup>	10.3	4.01	4.48
17 $\alpha$ -ethynodiol (EE2)	57-63-6		296.41	11,3 <sup>(e)</sup>	7.9x10 <sup>-12</sup>	10.3	3.67	2.71
Ibuprofen (IBU)	15687-27-1		206.29	21 <sup>(a)</sup>	1.5x10 <sup>-7</sup>	4.91	3.97	3.53

References: pubchem.ncbi.nlm.nih.gov, www.chemicalbook.com, www.SigmaAldrich.com.

(a) at 25 °C; (b) at 20 °C; (c) at 37 °C; (d) at 27 °C; (e) silt - sandy loam soils

**Table S2.** HPLC-DAD-FLD limit of detection and quantification.

Sample	Compound (abbreviation)	HPLC-DAD-FLD (mg/L)		
		LD*	LQ**	R <sup>2</sup>
S1 and S2	Caffeine	0.37	1.10	0.9991
	Carbamazepine	0.55	1.64	0.9986
	Oxybenzone	0.44	1.32	0.9993
S3	Caffeine (CAF)	0.13	0.40	0.9995
	Carbamazepine (CBZ)	0.09	0.26	0.9995
	Diclofenac (DCF)	0.18	0.54	0.9985
	Oxybenzone (OXY)	0.17	0.5	0.9996
	Triclosan (TCS)	0.33	0.99	0.9987
	Bisphenol A (BPA)	0.11	0.34	0.9999
	17 $\beta$ -estradiol (E2)	0.08	0.24	1.000
	17 $\alpha$ -ethinylestradiol (EE2)	0.14	0.42	0.9999
	Ibuprofen (IBU)	0.27	0.82	0.9996

\* limit of detection ; \*\* limit of quantification