

Supplementary Materials

# Occurrence of selected emerging contaminants in Southern Europe WWTPs: comparison of simulations and real data

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**Table S1.** Physicochemical characteristics of selected emerging compounds analysed in the present work.

Compound.	Type	Molecular weight (g/mol)	Solubility (mg/L)	Vapor pressure (Pa)	K <sub>ow</sub>	pKa	Henry coefficient (Pa·m <sup>3</sup> ·mol <sup>-1</sup> )
Ibuprofen	Acid	206.28	21	6.3·10 <sup>-3</sup>	9,332.54	4.52	0.015
Diclofenac	Acid	296.1	2.37	8.19·10 <sup>-6</sup>	32,359.37	4.15	4.79·10 <sup>-7</sup>
Erythromycin	Base	733.9	2000	2.83·10 <sup>-23</sup>	1,148.15	8.8	-
Triclosan	Neutral	289.5	10	6.13·10 <sup>-4</sup>	57,543.99	7.9	2.13·10 <sup>-3</sup>
Imidacloprid	Base	255.66	610	4·10 <sup>-10</sup>	3.715	11.12	1.67·10 <sup>-10</sup>
17α-ethinylestra-diol	Base	296.4	11.3	2.6·10 <sup>-7</sup>	4,677.35	10.33	8.05·10 <sup>-7</sup>

**Table S2.** Physicochemical and biological parameters provided by WWTP 1. BOD, biological oxygen demand; TTS, total suspended solids (INF: influent water after screening; TER: influent tertiary treatment); MLSSLM, mixed liquor suspended solids suspended within the mixed liquor.

Months	Treated flow (m <sup>3</sup> /day)	Average daily temperature (K)	pH	BOD (mg/L)	TSS <sub>INF</sub> (mg/L)	TSS <sub>TER</sub> (mg/L)	MLSS (mg/L)
July '20	3059	297.95	7.2	565	399	8	2448
August '20	2848	297.45	7.1	542	363	9	2730
September '20	2652	293.05	7.1	539	517	8	2925
October '20	2510	288.85	7.1	405	265	5	3404
November '20	2515	282.85	7.0	781	704	7	3014
December '20	2269	280.05	6.8	599	602	6	3899
January '21	3015	279.25	7.0	838	798	10	3477
February '21	2390	280.25	6.6	860	636	5	3338
March '21	3000	282.95	6.8	871	661	4	2943

**Table S3.** Physicochemical and biological parameters provided by WWTP 2. BOD, biological oxygen demand; TTS, total suspended solids (INF: influent water after screening; TER: influent tertiary treatment); MLSS, mixed liquor suspended solids suspended within the mixed liquor.

Months	Treated flow (m <sup>3</sup> /day)	Average daily temperature (K)	pH	BOD (mg/L)	TSS <sub>INF</sub> (mg/L)	TSS <sub>TER</sub> (mg/L)	MLSS (mg/L)
July '20	1706	298.75	7.8	428	385	14	2059
August '20	1647	299.15	7.8	532	377	9	2187
September '20	1704	294.25	7.7	410	346	11	2355
October '20	1761	289.35	7.4	385	380	15	2384
November '20	1944	286.05	7.5	404	291	9	2248
December '20	1842	282.75	7.5	362	306	9	2870
January '21	2368	281.45	7.5	403	283	11	3717
February '21	1793	284.55	7.6	415	373	10	3349
March '21	2123	284.15	7.6	449	339	10	2750

**Table S4.** Physicochemical and biological parameters provided by WWTP 3. BOD, biological oxygen demand; TTS, total suspended solids (INF: influent water after screening; TER: influent tertiary treatment); MLSS, mixed liquor suspended solids suspended within the mixed liquor.

Months	Treated flow (m <sup>3</sup> /day)	Average daily temperature (K)	pH	BOD (mg/L)	TSS <sub>INF</sub> (mg/L)	TSS <sub>TER</sub> (mg/L)	MLSS (mg/L)
July '20	4981	301.05	7.6	388	328	11	1378
August '20	4089	301.75	7.6	292	475	16	1013
September '20	4803	297.55	7.3	433	391	10	1166
October '20	4707	292.15	7.8	462	556	7	975
November '20	4936	289.35	7.5	297	346	6	1174
December '20	4672	285.15	7.4	470	410	4	996
January '21	4374	284.05	7.5	547	406	7	1923
February '21	4584	287.25	7.5	472	501	7	1366
March '21	4510	286.95	7.5	465	392	5	1123

**Table S5.** Physicochemical and biological parameters provided by WWTP 4. BOD, biological oxygen demand; TTS, total suspended solids (INF: influent water after screening; TER: influent tertiary treatment); MLSS, mixed liquor suspended solids suspended within the mixed liquor.

Months	Treated flow (m <sup>3</sup> /day)	Average daily temperature (K)	pH	BOD (mg/L)	TSS <sub>INF</sub> (mg/L)	TSS <sub>TER</sub> (mg/L)	MLSS (mg/L)
July '20	3450	297.75	7.77	441	382	7	1047
August '20	2239	297.15	7.8	529	506	4	1068
September '20	2185	292.65	7.81	638	407	9.3	1020
October '20	2087	288.35	7.86	439	454	9	1036
November '20	1385	282.25	7.86	575	685	16	1668
December '20	1714	279.55	8.02	575	505	16	1168
January '21	1710	278.75	7.81	478	752	19	1421

February '21	1536	279.75	7.88	560	425	11	1439
March '21	2128	282.45	7.88	530	635	10	1757

**Table S6.** Ibuprofen concentrations ( $\mu\text{g/L}$ ) and removal efficiencies (%) in influent and effluent in the four WWTPs analysed; n.d. is not detected.

Months	INFLUENT ( $\mu\text{g/L}$ )				EFFLUENT ( $\mu\text{g/L}$ )				Removal efficiency (%)			
	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4
July '20	2.92	8.42	4.35	6.53	0.03	0.04	0.09	0.84	99.0	99.5	97.9	87.1
August '20	1.70	2.72	3.12	2.48	0.08	0.01	0.04	0.07	95.3	99.6	98.7	97.2
September '20	1.70	1.56	3.11	1.41	0.27	n. d.	0.03	0.10	84.1	-	99.0	92.9
October '20	4.31	59.00	31.80	51.20	0.01	0.13	0.49	2.83	99.8	99.8	98.5	94.5
November '20	0.20	5.20	7.21	11.70	0.04	2.80	0.04	0.11	80.0	46.2	99.4	99.1
December '20	2.51	8.20	5.93	3.06	0.04	0.02	0.02	0.43	98.4	99.8	99.7	85.9
January '21	3.84	8.65	7.33	9.57	0.10	0.01	0.25	0.52	97.4	99.9	96.6	94.6
February '21	1.47	3.69	3.23	3.69	0.01	0.01	0.13	0.18	99.3	99.7	96.0	95.1
March '21	5.31	11.50	19.70	8.53	0.12	0.06	0.31	0.53	97.7	99.5	98.4	93.8

**Table S7.** Diclofenac concentrations ( $\mu\text{g/L}$ ) and removal efficiencies (%) in influent and effluent in the four WWTPs analysed; n.d. is not detected.

Months	INFLUENT ( $\mu\text{g/L}$ )				EFFLUENT ( $\mu\text{g/L}$ )				Removal efficiency (%)			
	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4
July '20	0.68	0.17	0.36	0.94	0.15	n. d.	0.26	n. d.	77.9	-	27.8	-
August '20	1.49	1.29	0.74	1.60	0.33	0.17	n. d.	n. d.	77.9	86.8	-	-
September '20	0.13	0.26	0.58	0.18	n. d.	n. d.	n. d.	n. d.	-	-	-	-
October '20	0.51	2.91	2.11	2.44	n. d.	1.32	0.95	3.66	-	54.6	55.0	-
November '20	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
December '20	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
January '21	0.84	0.29	0.61	2.64	1.04	0.41	1.15	2.01	-	-	-	23.9
February '21	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
March '21	n. d.	n. d.	n. d.	n. d.	0.24	n. d.	n. d.	n. d.	-	-	-	-

**Table S8.** Erythromycin concentrations ( $\mu\text{g/L}$ ) and removal efficiencies (%) in influent and effluent in the four WWTPs analysed; n.d. is not detected.

Months	INFLUENT ( $\mu\text{g/L}$ )				EFFLUENT ( $\mu\text{g/L}$ )				Removal efficiency (%)			
	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4
July '20	4.08	2.00	n. d.	4.21	n. d.	1.43	n. d.	1.13	-	28.5	-	73.2
August '20	22.90	10.80	77.90	39.20	3.40	45.8	8.89	n. d.	85.2	-	88.6	-
September '20	65.60	46.50	48.40	25.00	11.90	12.10	4.60	5.85	81.9	74.0	90.5	76.6
October '20	n. d.	1.29	1.52	0.39	n. d.	n. d.	n. d.	n. d.	-	-	-	-
November '20	n. d.	n. d.	171.00	29.70	n. d.	n. d.	25	n. d.	-	-	85.4	-
December '20	n. d.	n. d.	n. d.	7.66	n. d.	n. d.	n. d.	n. d.	-	-	-	-
January '21	n. d.	0.95	n. d.	0.61	n. d.	n. d.	0.09	n. d.	-	-	-	-
February '21	1.25	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
March '21	2.61	1.84	n. d.	0.67	0.84	1.13	0.61	n. d.	67.8	38.6	-	-

**Table S9.** Triclosan concentrations ( $\mu\text{g/L}$ ) and removal efficiencies (%) in influent and effluent in the four WWTPs analysed; n.d. is not detected.

Months	INFLUENT ( $\mu\text{g/L}$ )				EFFLUENT ( $\mu\text{g/L}$ )				Removal efficiency (%)			
	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4	WWTP 1	WWTP 2	WWTP 3	WWTP 4
July '20	0.04	0.03	0.01	0.01	n. d.	0.01	n. d.	0.01	-	66.7	-	0
August '20	0.19	0.20	0.20	0.21	0.18	0.20	0.19	0.19	5.3	0	5	9.5
September '20	0.02	0.04	0.04	0.01	0.01	0.03	0.02	0.02	50	25	50	-
October '20	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.02	0	0	50	-
November '20	n. d.	0.21	0.07	0.11	0.06	0.16	0.07	n. d.	-	23.8	0	-
December '20	n. d.	0.08	0.06	0.06	0.06	n. d.	n. d.	0.07	-	-	-	-
January '21	0.01	0.02	0.01	0.01	0.003	0.004	0.006	0.003	73.1	77.0	40	65.2
February '21	n. d.	0.24	0.07	0.10	n. d.	n. d.	n. d.	0.07	-	-	-	30.3
March '21	n. d.	0.04	0.03	0.01	n. d.	0.01	n. d.	n. d.	-	75	-	-

**Table S10.** Imidacloprid concentrations ( $\mu\text{g/L}$ ) and removal efficiencies (%) in influent and effluent in the four WWTPs analysed; n.d. is not detected.

Months	INFLUENT ( $\mu\text{g/L}$ )				EFFLUENT ( $\mu\text{g/L}$ )				Removal efficiency (%)			
	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP
	1	2	3	4	1	2	3	4	1	2	3	4
July '20	n. d.	0.04	0.06	n. d.	n. d.	0.05	n. d.	n. d.	-	-	-	-
August '20	0.46	0.85	0.40	0.56	0.35	0.33	0.38	0.33	23.9	61.2	5	41.1
September '20	0.53	1.05	0.31	0.41	0.11	0.49	0.11	0.24	79.2	53.3	64.5	41.5
October '20	3.23	9.91	14.1	3.36	4.11	7.80	4.56	3.27	-	21.3	67.7	2.7
November '20	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
December '20	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
January '21	n. d.	n. d.	n. d.	n. d.	0.09	n. d.	0.09	n. d.	-	-	-	-
February '21	0.13	n. d.	0.13	0.26	n. d.	n. d.	0.06	0.05	-	-	50.8	81.9
March '21	n. d.	0.65	0.66	0.57	0.49	0.48	0.53	n. d.	-	26.2	19.7	-

**Table S11.**  $17\alpha$ -ethinylestradiol concentrations ( $\mu\text{g/L}$ ) and removal efficiencies (%) in influent and effluent in the four WWTPs analysed; n.d. is not detected.

Months	INFLUENT ( $\mu\text{g/L}$ )				EFFLUENT ( $\mu\text{g/L}$ )				Removal efficiency (%)			
	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP
	1	2	3	4	1	2	3	4	1	2	3	4
July '20	0.19	0.21	0.02	0.10	n. d.	n. d.	n. d.	n. d.	-	-	-	-
August '20	0.26	0.25	0.37	0.27	n. d.	0.11	0.12	n. d.	-	56	67.6	-
September '20	0.02	0.01	0.01	0.02	0.003	0.003	0.002	0.003	85	70	80	85
October '20	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
November '20	0.83	1.04	0.1	0.25	0.09	n. d.	0.09	n. d.	89.2	-	10	-
December '20	0.37	0.26	0.09	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
January '21	0.14	0.18	0.02	0.06	0.001	n. d.	n. d.	n. d.	99.3	-	-	-
February '21	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-
March '21	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	-	-	-	-

**Table S12.** Biodegradation constant ( $k_i$ ) for ibuprofen, diclofenac and erythromycin in the four WWTPs analysed.

Months	$k_i$ Ibuprofen ( $h^{-1}$ )				$k_i$ Diclofenac ( $h^{-1}$ )				$k_i$ Erythromycin ( $h^{-1}$ )			
	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP
	1	2	3	4	1	2	3	4	1	2	3	4
July '20	2.94	36	1.48	0.194	0.1077	-	-	-	-	-	-	0.066
August '20	0.515	41	2.68	0.97	0.0891	0.69	-	-	0.141	-	0.272	-
September '20	0.1175	-	3.5	0.387	-	-	-	-	0.096	0.262	0.340	0.085
October '20	7.7	77	2.77	0.476	-	0.124	0.051	-	-	-	-	-
November '20	0.0814	-	6.2	1.27	-	-	-	-	-	-	0.212	-
December '20	0.96	69	13.5	0.1233	-	-	-	-	-	-	-	-
January '21	0.8	133	0.563	0.293	-	-	-	-	-	-	-	-
February '21	3.27	39	0.702	0.288	-	-	-	-	-	-	-	-
March '21	1.08	33.5	2.15	0.292	-	-	-	-	-	-	-	-

**Table S13.** Theoretical biodegradation constant ( $k_i$ ) for triclosan, imidacloprid and 17 $\alpha$ -ethinylestradiol in the four WWTPs analysed.

Months	$k_i$ Triclosan ( $h^{-1}$ )				$k_i$ Imidacloprid ( $h^{-1}$ )				$k_i$ 17 $\alpha$ -ethinylestradiol ( $h^{-1}$ )			
	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP	WWTP
	1	2	3	4	1	2	3	4	1	2	3	4
July '20	-	0.1250	-	-	-	-	-	-	-	-	-	-
August '20	-	-	-	-	0.0078	0.164	0.0015	0.0192	-	-	0.071	-
September '20	-	-	0.0015	-	0.085	0.114	0.0655	0.0197	0.124	0.223	0.1420	0.162
October '20	-	-	-	-	-	0.0274	0.088	0.0005	-	-	-	-
November '20	-	-	-	-	-	-	-	-	0.166	-	-	-
December '20	-	-	-	-	-	-	-	-	-	-	-	-
January '21	0.0179	0.225	-	0.016	-	-	-	-	3	-	-	-
February '21	-	-	-	-	-	-	0.03	0.067	-	-	-	-
March '21	-	0.255	-	-	-	0.0372	0.0083	-	-	-	-	-

**Table S14.** Biodegradation constant ( $k_{ib}$ ) obtained using Arrhenius equation for ibuprofen in the four WWTPs analysed.

Months	WWTP 1		WWTP 2		WWTP 3		WWTP 4	
	Daily T (K)	$k_{ib}$ ( $h^{-1}$ )	Daily T (K)	$k_{ib}$ ( $h^{-1}$ )	Daily T (K)	$k_{ib}$ ( $h^{-1}$ )	Daily T (K)	$k_{ib}$ ( $h^{-1}$ )
July '20	297.95	1.32	298.75	1.36	301.05	1.48	297.75	1.31
August '20	297.45	1.30	299.15	1.38	301.75	1.52	297.45	1.30
September '20	293.05	1.10	294.25	1.15	297.55	1.30	293.05	1.10
October '20	288.85	0.93	289.35	0.95	292.15	1.06	288.85	0.93
November '20	282.85	0.73	286.05	0.84	289.35	0.95	282.85	0.73
December '20	280.05	0.65	282.75	0.73	285.15	0.81	280.05	0.65
January '21	279.25	0.63	281.45	0.69	284.05	0.77	279.25	0.63
February '21	280.25	0.66	284.55	0.79	287.25	0.88	280.25	0.66
March '21	292.95	1.10	284.15	0.77	286.95	0.87	282.95	0.74

**Table S15.** Biodegradation constant ( $k_{di}$ ) obtained using Arrhenius equation for diclofenac in the four WWTPs analysed.

	WWTP 1		WWTP 2		WWTP 3		WWTP 4	
Months	Daily T (K)	$k_{di}$ (h <sup>-1</sup> )	Daily T (K)	$k_{di}$ (h <sup>-1</sup> )	Daily T (K)	$k_{di}$ (h <sup>-1</sup> )	Daily T (K)	$k_{di}$ (h <sup>-1</sup> )
July '20	297.95	0.18	298.75	0.20	301.05	0.26	297.75	0.18
August '20	297.45	0.17	299.15	0.21	301.75	0.28	297.45	0.17
September '20	293.05	0.10	294.25	0.12	297.55	0.17	293.05	0.10
October '20	288.85	0.06	289.35	0.07	292.15	0.09	288.85	0.06
November '20	282.85	0.03	286.05	0.05	289.35	0.07	282.85	0.03
December '20	280.05	0.02	282.75	0.03	285.15	0.04	280.05	0.02
January '21	279.25	0.02	281.45	0.03	284.05	0.04	279.25	0.02
February '21	280.25	0.02	284.55	0.04	287.25	0.05	280.25	0.02
March '21	292.95	0.10	284.15	0.04	286.95	0.05	282.95	0.03

**Table S16.** Biodegradation constant ( $k_{er}$ ) obtained using Arrhenius equation for erythromycin in the four WWTPs analysed.

	WWTP 1		WWTP 2		WWTP 3		WWTP 4	
Months	Daily T (K)	$k_{er}$ (h <sup>-1</sup> )	Daily T (K)	$k_{er}$ (h <sup>-1</sup> )	Daily T (K)	$k_{er}$ (h <sup>-1</sup> )	Daily T (K)	$k_{er}$ (h <sup>-1</sup> )
July '20	297.95	0.17	298.75	0.20	301.05	0.26	297.75	0.18
August '20	297.45	0.17	299.15	0.21	301.75	0.28	297.45	0.17
September '20	293.05	0.15	294.25	0.12	297.55	0.17	293.05	0.10
October '20	288.85	0.13	289.35	0.07	292.15	0.09	288.85	0.06
November '20	282.85	0.11	286.05	0.05	289.35	0.07	282.85	0.03
December '20	280.05	0.10	282.75	0.03	285.15	0.04	280.05	0.02
January '21	279.25	0.10	281.45	0.03	284.05	0.04	279.25	0.02
February '21	280.25	0.10	284.55	0.04	287.25	0.05	280.25	0.02
March '21	292.95	0.15	284.15	0.04	286.95	0.05	282.95	0.03