Supplementary Information

Elimination of micropollutants in activated sludge reactors with a special focus on the effect of biomass concentration

Rana Hatoum[1,2,3], Olivier Potier[1], Thibault Roques-Carmes[1], Cécile Lemaitre[1], Tayssir Hamieh[2], Joumana Toufaily[2], Harald Horn[3,4] and Ewa Borowska[3,*]

1. Laboratoire Réactions et Génie des Procédés, UMR CNRS 7274, University of Lorraine, Grandville 1, 54001 Nancy and France
2. Laboratory of Materials, Catalysis, Environment and Analytical Methods, Faculty of Sciences I, Lebanese University, Campus Rafic Hariri, Beirut, Lebanon
3. Engler-Bunte-Institut, Water Chemistry and Water Technology, Karlsruhe Institute of Technology (KIT), Engler-Bunte-Ring 9, 76131 Karlsruhe, Germany
4. DVGW Research Laboratories, Water Chemistry and Water Technology, Engler-Bunte-Ring 9, 76131 Karlsruhe, Germany

*Corresponding author. e-mail: ewa.borowska@kit.edu - Tel.: +49 721 608 42788; Fax: +49 721 608-46497

Table S1. Overview of the removal efficiency of some MPs in published studies according to some operational conditions in activated sludge.

HRT / SRT	Feed concentration (µg L^{-1})							Removal efficiency (%)							Sludge concentration (g_{TSS} L^{-1})
	CAF	SMX	BZT	ROX	ERY	DCF	CBZ	CAF	SMX	BZT	ROX	ERY	DCF	CBZ	
>2-3 / >150d (nitrifying conditions)[a]						≤1							70[b]		
12-17h / 1.5–5.1d[c]								44-75						8-15	
16.7h / 6d[d]	1	1				1	1	99	90				20	<10	2.4
58.4h / 54d[d]	1	1				1	1	95	45				10	<10	2.5
15h / 10-12d[e]		0.23-0.57							9		25	2			3
31h / 21-25d[e]		0.23-0.57							60						3
- / 20-40d, >40d[f]							10-40							<20	$2g_{VSS}$ L^{-1}
- / 20-40d, >40d[f]						10-40							<20		$2g_{VSS}$ L^{-1}
- / >40d[f]		10-40							64-70		64-70	64-70			$2g_{VSS}$ L^{-1}
12-20h / 25d[g]		1-5	1-5			1-5	1-5		20-90[h]				<20[g]	<20[g]	
12-20h / 40d[g]		1-5	1-5			1-5	1-5		20-90[h]				<20[g]	<20[g]	4-5.5
12-20h / 80d[g]		1-5	1-5			1-5	1-5		20-90[h]				<20[g]	<20[g]	4-5.5
12h / 3d[i]							0.24							--	
12.5-13.6 / 52-114d[i]							0.32-1.85							--	

[a]Vieno and Sillanpää [1]; [b]Fernandez-Fontaina et al. [2] ; [c]Santos et al. [3] ; [d]Majewsky et al. [4] ; [e]Gobel et al. [5] ; [f]Suárez et al. [6] ; [g]Falås et al. [7] [h]Joss et al. [8] [i]Hai et al. [9]. / --negligeable.

Table S2. Operating schedule of SBRs.

	Operating times in each cycle								
	SRT (d)	**HRT (h)***	**Duration (d)****	**Filling (min)**	**Reaction (min)**	**Settling (min)**	**Drawing (min)**	**# of cyles (d^{-1})**	**Treated wastewater (L d^{-1})**
SBR-3 d	3	4	30	5	170	60	5	6	30
		8	30	5	410	60	5	3	15
		12	30	5	650	60	5	2	10
SBR-10 d	10	4	30	5	170	60	5	6	30
		8	30	5	410	60	5	3	15
		12	30	5	650	60	5	2	10
SBR-20 d	20	4	30	5	170	60	5	6	30

*: Studied HRT is equivalent to the cycle duration; **: Actual kinetics periods. These periods include transition period between phases.

Table S3. Mean values of biomass concentration (± standard error), volatile suspended solids (VSS), dissolved oxygen (DO), pH and T (°C) in the three SBRs during seven experimental setups.

SRT (d)	**3**	**3**	**3**	**10**	**10**	**10**	**20**
HRT (h)	4	8	12	4	8	12	4
Biomass concen-tration (g L^{-1})	3.3 ± 0.1	3.3 ± 0.1	3.2 ± 0.1	3.0 ± 0.1	3.3 ± 0.1	3.1 ± 0.1	3.5 ± 0.1
VSS (%)	70	72	71	79	77	79	81
DO (mg L^{-1})	2.5	2.4	2.2	4.4	4.3	4.2	4.4
pH	8.1	8.1	8	7.5	7.8	7.9	8
T (°C)	20.1	19	19	18.1	18	18	19.5

Table S4. Composition of the synthetic wastewater and supplementary solutions I and II.

Synthetic wastewater (SWW)	**Concentration (mg L^{-1})**		
	SWW1 (SBR-3 d)	SWW2 (SBR-10 d)	SWW3 (SBR-20 d)
CH_3COONa	1200	500	100
NH_4HCO_3	75	75	75
KH_2PO4	5	5	5
$MgSO_4.7H_2O$	50	50	50
$CaCl_2.2H_2O$	21	21	21
$NaHCO_3$	36	36	36
Supplementary solution I			
$C_{10}H_6N_2O_8$	50	50	5
$FeSO_4.7H_2O$	20	20	2
Supplementary solution II			
$C_{10}H_6N_2O_8$	20	20	20
$ZnSO_4.7H_2O$	0.43	0.43	0.43
$CoCl_2.6H_2O$	0.24	0.24	0.24
$MnCl_2.4H_2O$	1	1	1
$CuSO_4.5H_2O$	0.25	0.25	0.25
$NaMoO_4.2H_2O$	0.22	0.22	0.22
$NiCl_2.6H_2O$	0.19	0.19	0.19
$NaSeO_4.10H_2O$	0.21	0.21	0.21
H_3BO_4	0.14	0.14	0.14

Text S1. Calculation of Solid Retention Time (SRT).The target SRTs were maintained manually by adjustment of biomass concentration in SBRs at the end of the aeration period according to reference [10] using the Eq. (S1):

$$SRT = \frac{C_{\mathrm{TSS}}\,\mathrm{V}}{C_{\mathrm{TSS}\ eff}\,Q_{eff} + C_{\mathrm{TSS}\ w}\,\mathrm{Q}_w} \quad \text{(S1)} \qquad (1)$$

where C_{TSS}: Total Suspended Solids concentration in the reactor (g_{TSS} L^{-1}); V: reactor volume (L); C_{TSSeff} : Total Suspended Solids concentration in the effluent (g TSS L^{-1});$Q_{eff.}$: effluent flow rate (L d^{-1}); C_{TSSw}: Total Suspended Solids concentration of the withdrawn sludge (g TSS L^{-1});Q_w: sludge withdrawal (L d^{-1}).

Table S5. Source parameters applied during sample measurements.

Source parameters	
Gas Temperature	200 ^{0}C
Gas Flow	8 L min^{-1}
Nebulizer	40 psi
Sheath Gas Temperature	300 ^{0}C
Sheath Gas Flow	12 L min^{-1}
Capillary	Positive: 4500 V Negative 3500 V
Nozzle Voltage	Positive 500 V Negative 300 V

Table S6. Mass spectrometric parameters for detection.

Compound	RT min	Polarity	Precursor Ion	Quantifier	CE	Qualifier	CE
Benzotriazole	3.3	Positive	120.1	65.0	24	92.1	20
Benzotriazole-d_4	3.3	Positive	124.1	41.4	48	96.0	20
Caffeine	3.0	Positive	195.1	137.9	20	110.0	24
Caffeine-$^{13}C_3$	3.0	Positive	198.2	140.0	20	43.5	44
Carbamazepine	5.8	Positive	237.1	193.4	28	178.9	40
Carbamazepine-d_8	5.8	Positive	245.2	202.1	24	200.6	40
Diclofenac	8.0	Positive	296.0	213.9	40	250.0	12
Diclofenac-d_4	8.0	Positive	300.1	218.0	36	-	-
		Negative	298.0	-	-	254.0	8
Erythromycin	3.6	Positive	734.5	158.0	32	576.0	20
Erythromycin-d_3	3.6	Positive	737.5	161.0	32	579.4	20
Roxithromycin	3.9	Positive	837.5	158.0	36	679.4	20
Roxithromycin-d_7	3.9	Positive	844.6	158.0	36	686.5	20
Sulfamethoxazole	4.4	Positive	254.1	155.9	12	92.0	28
Sulfamethoxazole-d_4	4.4	Positive	258.1	159.9	36	151.1	12

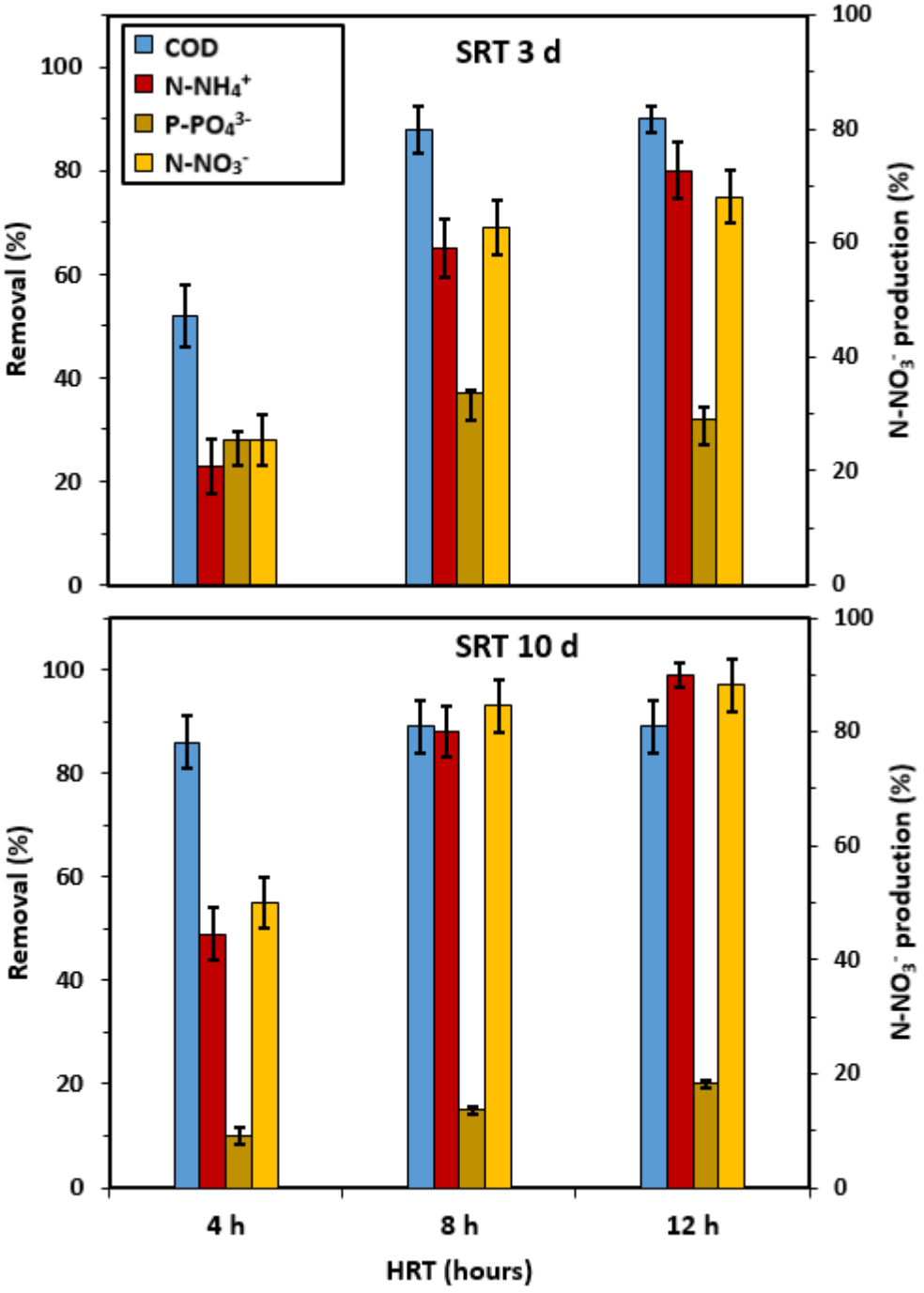

Figure S1. Removal efficiencies of wastewater parameters (COD, N-NH_4^+ and P-PO_4^{3-}) and nitrate-nitrogen production over 4 h, 8 h and 12 h HRT for SRT - 3 d and SRT - 10 d (error bars present standard error).

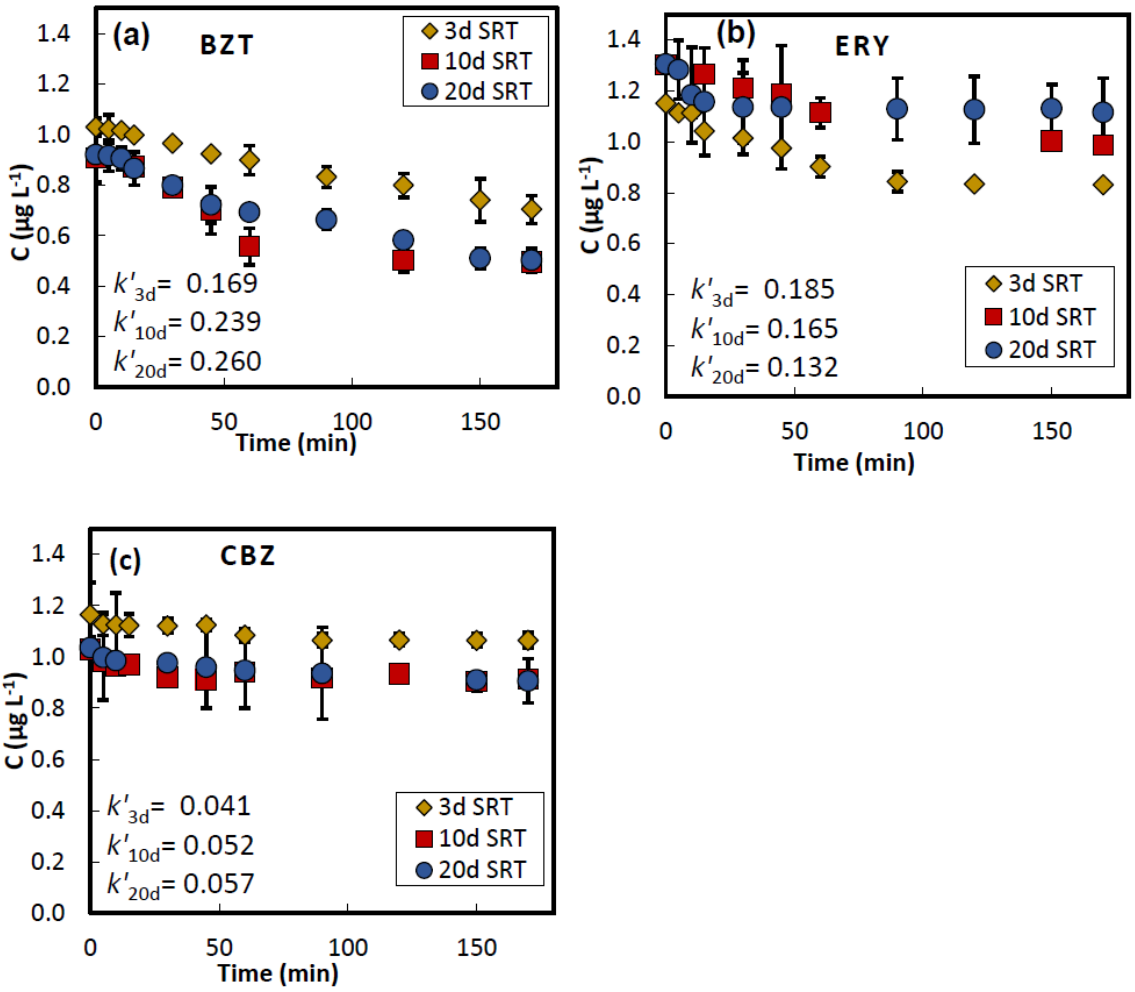

Figure S2. Removal and k′: apparent-first-order fits (h^{-1}) of other investigated MPs; number of replicates = 3; error bars indicate one standard error.

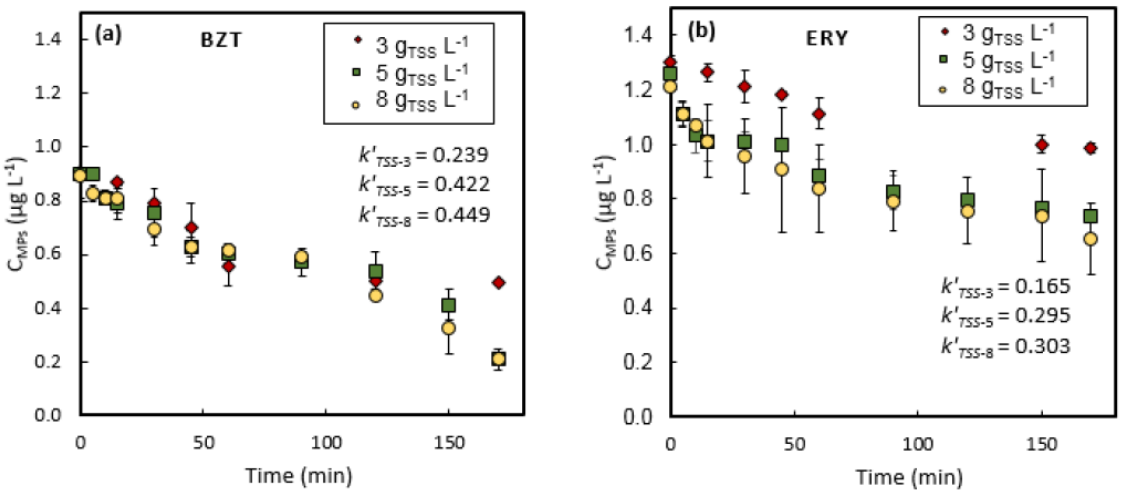

Figure S3. Change of concentration of (a) BZT and (b) ERY during biological treatment in reactors inoculated with biomass at concentrations of 3, 5 and 8 g L^{-1}; k′: apparent-first-order removal rate constant (h^{-1}) at SRT - 10 d and HRT - 4 h.

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