

Supplementary Material

Accurate detection and quantification of nineteen micropollutants by online SPE-LC-MS/MS method in raw and biologically treated wastewater: assessment of mobile phase composition and matrix effect

Rodrigo B. Carneiro^{a*}, Elis W. Nogueira^b, Carolina A. Sabatini^b, Marcelo Zaiat^b and Álvaro J. Santos-Neto^a

^a Laboratory of Chromatography (CROMA), São Carlos Institute of Chemistry (IQSC), University of São Paulo (USP), 400, Trabalhador São-Carlense Ave., São Carlos, São Paulo 13566-590, Brazil

e-mail: rodrigocarneiro@sc.usp.br; alvarojsn@iqsc.usp.br

^b Laboratory of Biological Processes (LPB), São Carlos School of Engineering, University of São Paulo (USP), 1100, João Dagnone Ave., Santa Angelina, 13563-120, São Carlos, São Paulo, Brazil.

e-mail: eliswn@usp.br; casm@sc.usp.br; zaiat@sc.usp.br

Corresponding author:

* rodrigocarneiro@sc.usp.br, Phone: +55 (16) 3373-8357 / 3373-8358;

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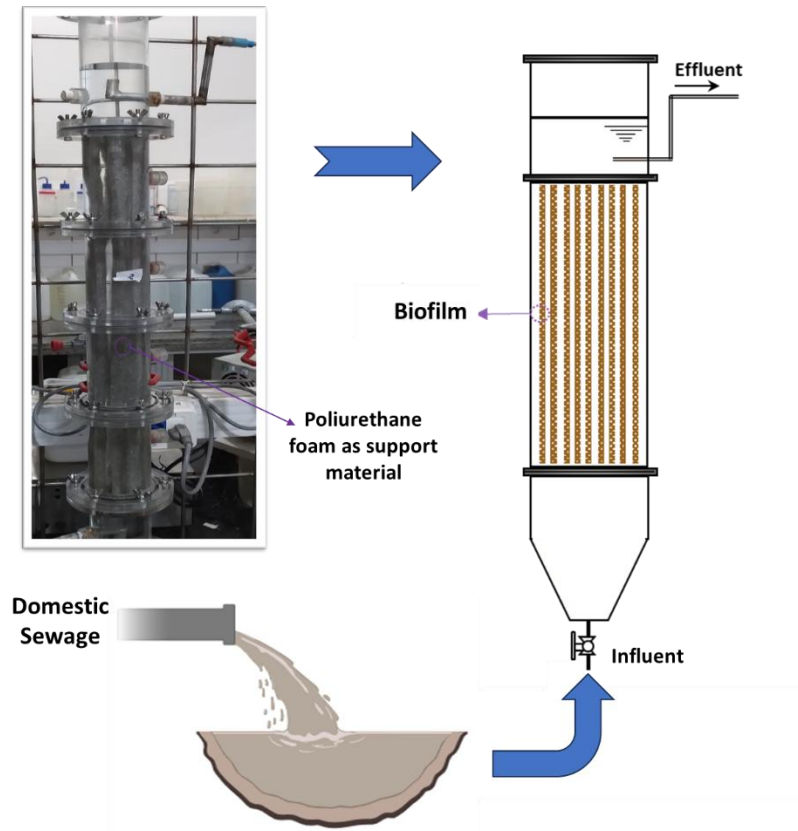


Figure S1. Experimental apparatus detailing the structure of the anaerobic fixed bed bioreactor (AnFBBR) with polyurethane foam as support material.

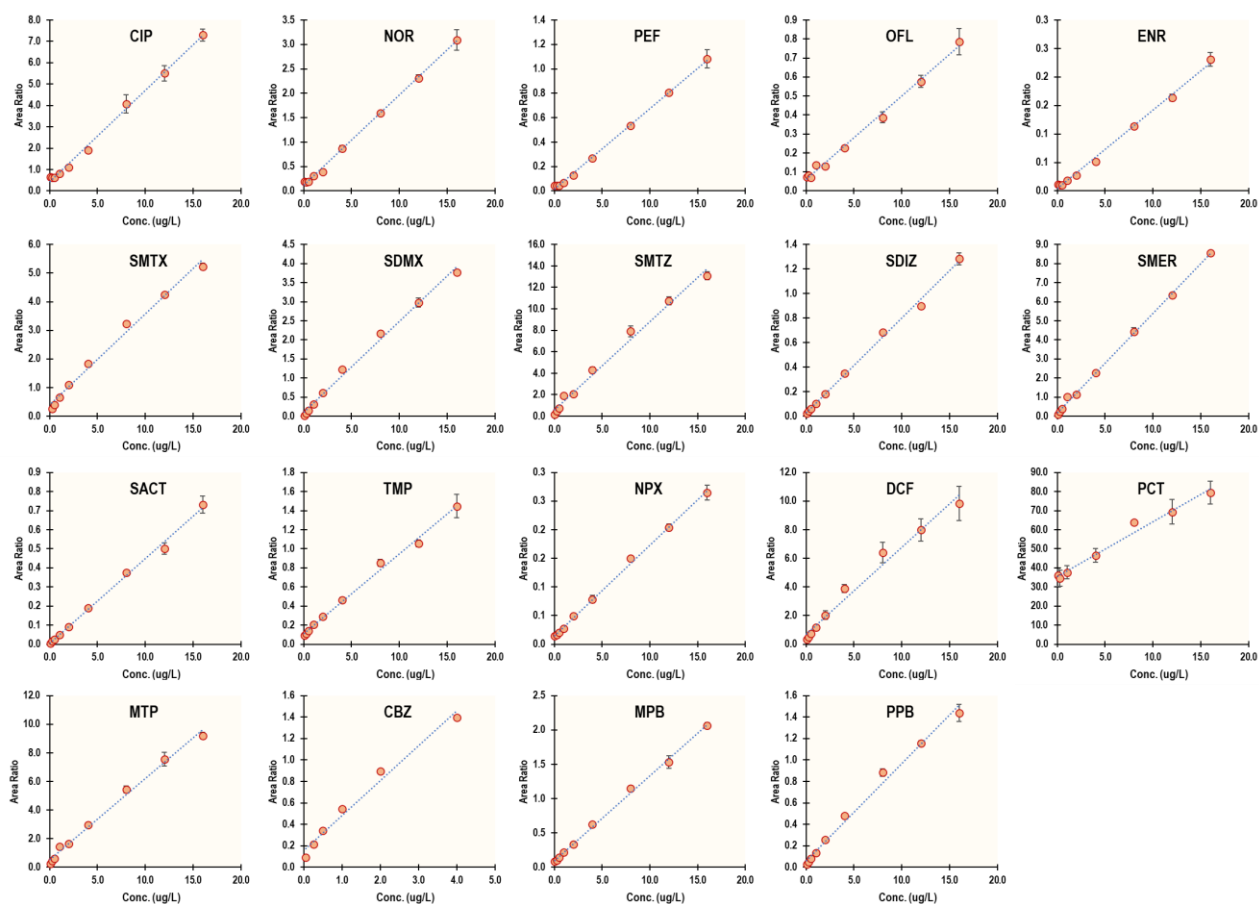


Figure S2. Calibration curves for the 19 target MPs spiked into the bioreactor influent matrix (domestic sewage)

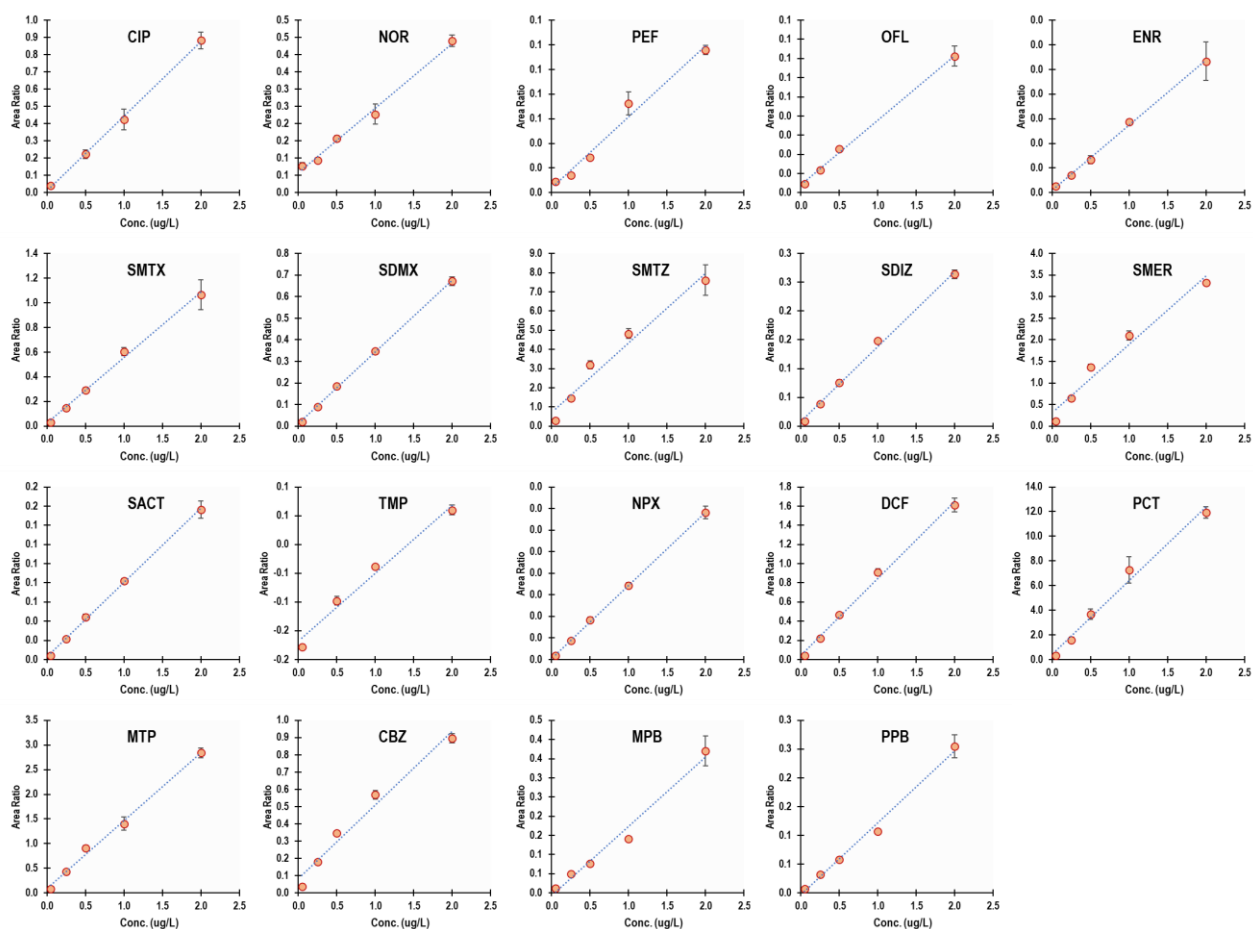


Figure S3. Calibration curves for the 19 target MPs spiked into the ultrapure water.

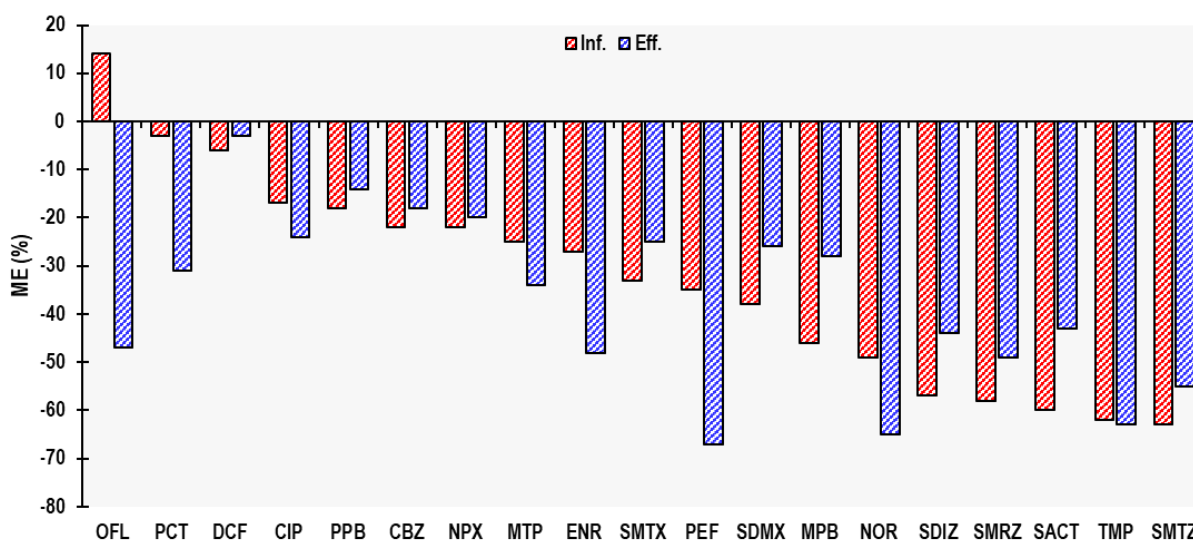


Figure S4. Mean matrix effect (ME) values (%) of the 19 target MPs spiked into the influent and effluent from the bioreactor.

Table S1. MS/MS parameters for the internal standards (IS) by SRM.

IS	Ionization mode	Precursor ion (m/z)	Product ion (m/z)	DP (V)	CE (eV)	CXP (V)
SMTX- ¹³ C	Positive	260	98 ^a	96	39	16
			114	96	39	16
			162	96	33	6
SDMX- ¹³ C	Positive	317	162 ^a	76	41	14
			114	76	41	16
			98	76	27	16
TMP-D ₉	Positive	300	234 ^a	106	35	12
			264	106	35	12
			123	106	35	12
CIP-D ₈	Positive	340	296 ^a	81	25	14
			249	81	25	14
NOR-D ₅	Positive	325	281 ^a	101	25	14
			238	101	25	14
ENR-D ₅	Positive	365	321 ^a	31	27	16
			245	91	55	9
			347	91	55	9
CBZ-D ₁₀	Positive	247	204 ^a	96	33	25
DCF-D ₄	Negative	298	254 ^a	100	20	12
NPX-D ₃	Negative	232	188 ^a	100	12	8
PCT-D ₃	Negative	153	107 ^a	100	32	18

^a quantification ion

Table S2 Chromatographic areas resulting from tests carried out with different mobile phases - acetonitrile (A), acetonitrile : methanol (50:50 v:v) (AM), methanol (M), and different additives - formic acid (FA) and ammonium hydroxide (AH)

Concentration level	MP ^a	FA ^b			AH ^f		
		A ^c	AM ^d	M ^e	A ^c	AM ^d	M ^e
16 µg L ⁻¹	OFL	8.1·10 ⁵	1.7·10 ⁶	1.4·10 ⁷	1.6·10 ⁶	3.7·10 ⁷	3.1·10 ⁷
	ENR	1.3·10 ⁷	1.8·10 ⁷	3.1·10 ⁶	1.6·10 ⁷	2.2·10 ⁷	2.7·10 ⁵
	PEF	5.4·10 ⁵	3.2·10 ⁶	1.6·10 ⁷	2.2·10 ⁶	4.1·10 ⁷	2.8·10 ⁷
	CIP	1.4·10 ⁷	6.1·10 ⁶	4.9·10 ⁷	6.9·10 ⁷	2.0·10 ⁷	9.1·10 ⁷
	TMP	3.0·10 ⁶	5.8·10 ⁷	5.5·10 ⁷	7.2·10 ⁷	7.2·10 ⁹	1.2·10 ⁸
	CBZ	6.5·10 ⁷	7.4·10 ⁷	9.2·10 ⁷	1.1·10 ⁸	8.0·10 ⁷	1.2·10 ⁸
	PCT	2.6·10 ⁶	2.8·10 ⁶	3.5·10 ⁶	7.9·10 ⁶	3.3·10 ⁶	1.6·10 ⁷
	NPX	1.1·10 ⁷	5.6·10 ⁶	4.4·10 ⁷	1.5·10 ⁶	9.4·10 ⁶	3.2·10 ⁷
	DCF	2.7·10 ⁶	2.6·10 ⁶	2.5·10 ⁶	1.1·10 ⁶	3.4·10 ⁶	1.4·10 ⁷
	MTP	3.9·10 ⁶	3.6·10 ⁷	3.4·10 ⁷	5.6·10 ⁷	5.6·10 ⁷	7.8·10 ⁷
	MPB	7.1·10 ⁶	3.4·10 ⁶	5.9·10 ⁶	6.8·10 ⁶	1.1·10 ⁷	1.7·10 ⁷
	PPB	1.9·10 ⁷	2.1·10 ⁷	1.9·10 ⁷	2.8·10 ⁷	9.4·10 ⁶	3.7·10 ⁷
0.5 µg L ⁻¹	OFL	4.4·10 ⁴	1.0·10 ⁵	2.6·10 ⁵	2.5·10 ⁴	1.0·10 ⁶	7.4·10 ⁶
	ENR	2.9·10 ⁵	5.4·10 ⁵	1.5·10 ⁵	4.3·10 ⁵	6.5·10 ⁵	6.1·10 ⁶
	PEF	2.9·10 ⁴	1.6·10 ⁵	3.8·10 ⁵	nd ^g	1.8·10 ⁶	9.4·10 ⁶
	CIP	4.0·10 ⁵	3.6·10 ⁵	1.8·10 ⁶	2.8·10 ⁶	9.2·10 ⁵	3.0·10 ⁷
	TMP	2.0·10 ⁵	9.5·10 ⁶	7.2·10 ⁶	8.6·10 ⁶	1.5·10 ⁷	1.1·10 ⁷
	CBZ	1.2·10 ⁷	1.3·10 ⁷	7.9·10 ⁶	2.2·10 ⁷	5.2·10 ⁶	2.3·10 ⁷
	PCT	1.7·10 ⁵	1.4·10 ⁵	2.1·10 ⁵	4.0·10 ⁵	1.2·10 ⁵	5.5·10 ⁵
	NPX	3.9·10 ⁵	2.6·10 ⁵	1.1·10 ⁶	1.4·10 ⁵	4.6·10 ⁵	2.5·10 ⁶
	DCF	2.5·10 ⁵	2.2·10 ⁵	1.9·10 ⁵	4.1·10 ⁵	1.8·10 ⁶	8.7·10 ⁶
	MTP	1.5·10 ⁵	3.3·10 ⁶	1.8·10 ⁶	2.4·10 ⁶	2.3·10 ⁶	2.7·10 ⁶
	MPB	4.0·10 ⁵	1.7·10 ⁵	2.5·10 ⁵	3.3·10 ⁵	3.1·10 ⁵	6.7·10 ⁵
	PPB	1.1·10 ⁶	1.0·10 ⁶	6.7·10 ⁵	1.6·10 ⁶	3.1·10 ⁵	1.2·10 ⁶

^a MP: micropollutant; ^b FA: formic acid; ^c A: acetonitrile; ^d AM: Acetonitrile + Methanol (50:50 v:v); ^e M: Methanol; ^f AH: Ammonium Hydroxide; ^g nd: not detected.

Table S3. pKa values for each MP and its respective dominant ionization state under each pH condition – acidic (formic acid, pH $\approx$ 3) and alkaline (ammonium hydroxide, pH $\approx$ 10), according to Chemicalize (<https://chemicalize.com/welcome>)

MP	pKa	Dominant state at pH 3 (FA)	Dominant state at pH 10 (AH)
SMTX	6.16	Neutral	Deprotonated (-)
SDMX	6.91	Neutral	Deprotonated (-)
SMTZ	6.99	Neutral	Deprotonated (-)
SDIZ	6.99	Neutral	Deprotonated (-)
SMRZ	6.99	Neutral	Deprotonated (-)
SACT	5.60	Neutral	Deprotonated (-)
TMP	7.16	Protonated (+)	Neutral
CIP	5.56	Protonated (+)	Deprotonated (-)
NOR	5.97	Protonated (+)	Deprotonated (-)
PEF	5.97	Protonated (+)	Deprotonated (-)
OFL	5.77	Protonated (+)	Deprotonated (-)
ENR	5.95	Protonated (+)	Deprotonated (-)
CBZ	15.96	Neutral	Neutral
MTP	9.27	Protonated (+)	Neutral
DCF	4.01	Neutral	Deprotonated (-)
NPX	4.19	Neutral	Deprotonated (-)
PCT	9.46	Neutral	Deprotonated (-)
MPB	8.50	Neutral	Deprotonated (-)
PPB	8.50	Neutral	Deprotonated (-)

Table S4. Validation parameters of the analytical method - retention time (R_t), limits of detection and quantification (LOD and LOQ), and linear determination coefficient (r^2) of the calibration curves in ultrapure water, influent and effluent matrices from the biological reactor.

MP	Rt (min)	Water			Influent			Effluent		
		LOD	LOQ	r^2	LOD	LOQ	r^2	LOD	LOQ	r^2
		(ng L ⁻¹)	(ng L ⁻¹)		(ng L ⁻¹)	(ng L ⁻¹)		(ng L ⁻¹)	(ng L ⁻¹)	
SMTX	6.40	20	68	0.980	12	39	0.989	22	74	0.989
SDMX	6.68	39	130	0.998	46	152	0.993	45	150	0.989
SMTZ	6.18	15	50	0.950	20	65	0.988	7	23	0.974
SDIZ	5.93	30	99	0.994	64	213	0.995	22	74	0.997
SMRZ	6.06	6	20	0.972	50	165	0.997	21	69	0.980
SACT	5.89	7	23	0.994	51	171	0.993	17	57	0.998
TMP	5.96	31	103	0.998	88	295	0.988	23	77	0.995
CIP	6.01	24	81	0.990	55	184	0.990	42	140	0.985
NOR	6.01	34	114	0.983	143	478	0.995	42	140	0.991
PEF	6.01	35	116	0.971	136	452	0.995	41	137	0.984
OFL	6.01	25	82	0.991	134	448	0.986	37	123	0.992
ENR	6.06	12	39	0.973	88	295	0.994	21	70	0.994
CBZ	7.17	29	96	0.972	49	164	0.981	23	77	0.989
MTP	6.17	23	77	0.990	78	260	0.990	13	45	0.976
DCF	10.18	5	17	0.992	51	169	0.963	11	38	0.971
NPX	8.12	18	59	0.997	95	316	0.996	33	109	0.996
PCT	5.82	6	20	0.974	46	152	0.933	11	37	0.989
MPB	6.68	14	45	0.968	23	77	0.996	14	47	0.996
PPB	7.62	2	5	0.985	82	273	0.988	17	58	0.993

Table S5. RSD values (%) for each concentration level of the calibration curves of the 19 target MPs spiked into the bioreactor influent matrix (domestic sewage)

Concentration levels ($\mu\text{g L}^{-1}$)	SMTX	CBZ	PCT	DCF	SDMX	ENR	CIP	NOR	OFL	PEF
0.05	5	1	8	8	4	1	6	1	10	1
0.25	1	2	12	14	4	7	15	3	2	2
0.5	8	1	6	10	5	3	4	8	6	12
1	3	2	9	7	4	1	6	1	2	4
2	1	2	10	14	6	5	10	7	5	3
4	3	1	8	7	3	6	7	6	3	5
8	1		2	11	1	4	11	2	8	3
12	3		9	10	4	4	7	3	6	2
16	2		8	12	1	5	4	7	9	7
Concentration levels ($\mu\text{g L}^{-1}$)	TMP	SACT	SDIZ	SMRZ	SMTZ	MTP	MPB	PPB	NPX	
0.05	2	5	6	8	3	3	5	2	1	
0.25	4	4	2	6	3	8	4	2	4	
0.5	3	4	5	1	1	4	6	6	4	
1	5	5	2	3	2	3	3	6	9	
2	5	3	1	4	4	6	2	3	1	
4	5	4	5	3	6	3	3	4	9	
8	4	2	1	4	6	5	1	4	2	
12	3	6	2	1	3	6	6	2	3	
16	8	6	4	1	3	2	2	5	5	

Table S6. RSD values (%) for each concentration level of the calibration curves of the 19 target MPs spiked into the bioreactor effluent matrix.

Concentration levels ($\mu\text{g L}^{-1}$)	SMTX	CBZ	PCT	DCF	SDMX	ENR	CIP	NOR	OFL	PEF
0.05	3	3	7	6	8	5	10	8	14	9
0.25	4	3	10	9	2	7	8	4	8	5
0.5	3	1	9	6	6	13	4	4	6	7
1	1	2	5	10	6	4	3	4	5	5
2	2	1	1	3	1	4	5	5	3	3
4	1	3	6	10	4	7	7	5	4	3
8	5		3	10	5	1	11	4	2	3
12	3		8	12	5	4	1	4	3	7
16	3		2	10	1	4	6	10	8	10
Concentration levels ($\mu\text{g L}^{-1}$)	TMP	SACT	SDIZ	SMRZ	SMTZ	MTP	MPB	PPB	NPX	
0.05	2	9	5	5	6	7	10	5	10	
0.25	6	2	6	2	4	5	2	5	4	
0.5	1	8	6	8	3	7	8	1	13	
1	2	5	7	2	5	4	5	4	9	
2	4	2	3	5	3	4	5	7	7	
4	5	3	2	7	3	4	4	2	13	
8	4	4	4	6	9	8	3	6	10	
12	4	4	5	3	5	2	5	3	9	
16	2	3	2	3	3	3	5	4	1	

Table S7. RSD values (%) for each concentration level of the calibration curves of the 19 target MPs spiked into the ultrapure water.

Concentration levels ($\mu\text{g L}^{-1}$)	SMTX	CBZ	PCT	DCF	SDMX	ENR	CIP	NOR	OFL	PEF
0.05	5	1	12	8	12	10	15	13	14	14
0.25	8	1	15	3	7	7	12	7	5	4
0.5	5	4	11	4	2	12	14	5	2	7
1	5	4	15	4	1	13	14	13	10	13
2	11	3	4	4	3	15	5	4	7	3
Concentration levels ($\mu\text{g L}^{-1}$)	TMP	SACT	SDIZ	SMRZ	SMTZ	MTP	MPB	PPB	NPX	
0.05	1	8	4	6	1	14	11	7	10	
0.25	1	4	3	3	3	5	4	1	7	
0.5	7	7	6	5	6	5	8	1	7	
1	8	3	2	5	5	10	2	2	4	
2	14	6	3	2	10	4	11	8	4	

Table S8. Relative recovery values (%) for five concentration levels of the 19 target MPs spiked into the influent and effluent matrices from the bioreactor.

Concentration levels ($\mu\text{g L}^{-1}$)	SMTX		CBZ		PCT		DCF		SDMX	
	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.
0.25	60	75	67	75	185	63	94	98	58	70
0.5	64	71	69	79	116	73	95	98	52	66
1	59	65	69	74	73	57	86	91	55	66
2	69	74	76	76	64	78	97	95	63	76
20	82	88	108	104	48	76	97	102	81	89
Average $\pm$ SD	67 $\pm$ 9	75 $\pm$ 8	78 $\pm$ 17	82 $\pm$ 13	97 $\pm$ 55	69 $\pm$ 9	94 $\pm$ 5	97 $\pm$ 4	62 $\pm$ 11	74 $\pm$ 10
Concentration levels ($\mu\text{g L}^{-1}$)	ENR		CIP		NOR		OFL		PEF	
	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.
0.25	28	46	94	95	12	15	109	29	35	17
0.5	62	58	88	93	32	25	103	68	42	25
1	26	34	31	61	30	31	82	47	21	33
2	116	61	103	56	76	40	170	69	107	39
20	131	62	100	73	107	62	106	55	121	51
Average $\pm$ SD	73 $\pm$ 49	52 $\pm$ 12	83 $\pm$ 30	76 $\pm$ 18	51 $\pm$ 39	35 $\pm$ 18	114 $\pm$ 33	53 $\pm$ 17	65 $\pm$ 46	33 $\pm$ 13
Concentration levels ($\mu\text{g L}^{-1}$)	TMP		SACT		SDIZ		SMRZ		SMTZ	
	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.
0.25	17	14	39	52	36	48	30	38	25	33
0.5	25	21	36	55	39	52	32	41	26	32
1	36	34	38	56	37	49	33	43	26	33
2	47	47	38	55	42	54	42	49	33	41
20	64	70	47	66	62	77	71	83	77	85
Average $\pm$ SD	38 $\pm$ 19	37 $\pm$ 22	40 $\pm$ 4	57 $\pm$ 5	43 $\pm$ 11	56 $\pm$ 12	42 $\pm$ 17	51 $\pm$ 19	37 $\pm$ 23	45 $\pm$ 23
Concentration levels ($\mu\text{g L}^{-1}$)	MTP		MPB		PPB		NPX			
	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.	Inf.	Eff.		
0.25	61	69	45	67	73	76	80	72		
0.5	63	72	56	76	91	94	74	83		
1	61	72	59	78	86	93	68	88		
2	68	71	49	66	76	77	88	74		
20	80	88	62	75	86	89	81	85		
Average $\pm$ SD	75 $\pm$ 7	66 $\pm$ 8	54 $\pm$ 7	72 $\pm$ 6	82 $\pm$ 7	86 $\pm$ 9	78 $\pm$ 8	80 $\pm$ 7		

Table S9. Concentrations (ng L⁻¹) of the 19 target MPs found in domestic sewage samples (Inf.) and anaerobic bioreactor effluent (Eff.).

MP	Matrix	Sample						Range (ng L ⁻¹)	Median (ng L ⁻¹)	Average (ng L ⁻¹)	Average Mass load (µg d ⁻¹)
		1	2	3	4	5	6				
SMTX	Inf.	37	20	46	31	26	32	20 – 46	31	32	0.13
	Eff.	nd	nd	nd	nd	nd	nd	<LOD	<LOD	<LOD	-
SDMX	Inf.	nd	nd	nd	nd	nd	nd	<LOD	<LOD	<LOD	-
	Eff.	nd	nd	nd	nd	nd	nd	<LOD	<LOD	<LOD	-
SMTZ	Inf.	34	29	35	34	38	34	29 – 38	34	34	0.14
	Eff.	11	9	10	12	12	16	9 – 16	11	12	0.05
SDIZ	Inf.	994	644	361	743	986	349	349 – 994	694	680	2.72
	Eff.	291	137	123	186	200	187	123 – 201	187	173	0.69
SMRZ	Inf.	281	255	280	154	283	295	154 – 295	281	258	1.03
	Eff.	81	68	58	56	69	59	56 – 81	63	65	0.26
SACT	Inf.	62	nd	nd	nd	nd	nd	<LOD – 62	<LOD	<LOD	-
	Eff.	nd	nd	nd	nd	nd	nd	<LOD	<LOD	<LOD	-
TMP	Inf.	375	105	273	145	205	153	105 – 375	179	209	0.84
	Eff.	41	nd	nd	nd	nd	nd	<LOD – 41	<LOD	<LOD	-
CIP	Inf.	1195	1106	525	2512	1102	1319	525 – 2512	1150	1293	5.17
	Eff.	535	231	180	457	362	585	180 – 585	409	392	1.57
NOR	Inf.	475	536	543	691	721	676	475 – 721	610	607	2.43
	Eff.	415	351	299	386	426	400	299 – 426	393	379	1.52
PEF	Inf.	318	418	273	732	414	350	273 – 732	382	418	1.67
	Eff.	269	258	201	659	299	270	201 – 659	269	326	1.30
OFL	Inf.	542	757	692	672	1477	667	542 – 1477	682	801	3.20
	Eff.	170	nd	nd	86	457	362	<LOD – 0.46	128	179	0.72
ENR	Inf.	348	415	317	337	436	394	317 – 436	371	374	1.50
	Eff.	69	99	60	158	154	199	60 – 199	126	123	0.49
CBZ	Inf.	210	347	152	166	166	196	152 – 347	181	206	0.82
	Eff.	185	308	127	134	139	157	127 – 308	148	175	0.70
MTP	Inf.	307	360	374	294	352	323	294 – 374	337	335	1.34
	Eff.	92	103	100	102	100	89	89 – 103	100	98	0.39
DCF	Inf.	222	227	237	364	350	350	222 – 364	293	291	1.16
	Eff.	212	216	231	284	320	335	212 – 335	257	266	1.06
NPX	Inf.	616	705	723	640	1167	1609	616 – 1609	714	910	3.64
	Eff.	359	508	365	338	548	949	338 – 949	437	511	2.04
PCT	Inf.	17366	19980	15722	11528	16776	12529	11528 – 19980	16249	15650	62.60
	Eff.	3541	2471	1578	1378	2025	1575	1378 – 3541	1802	2095	8.38
MPB	Inf.	769	397	423	631	980	907	397 – 980	700	684	2.74
	Eff.	nd	nd	21	nd	nd	nd	<LOD – 21	<LOD	<LOD	-
PPB	Inf.	418	178	200	424	270	379	178 – 424	324	312	1.25
	Eff.	nd	nd	nd	nd	nd	nd	<LOD	<LOD	<LOD	-

nd – Not detected; LOD – Limit of detection (Table S2)

Table S10. Maximum concentrations of MPs in the anaerobic reactor influent and effluent, and PNEC values used to calculate the Risk Quotient

MP	Conc. _{max} Inf. (µg L ⁻¹)	Conc. _{max} Eff. (µg L ⁻¹)	PNEC (µg L ⁻¹)	RQ _{inf}	RQ _{eff}	Risk Reduction (%)
SDIZ	0.99	0.20	1	0.994	0.201	80%
PCT	19.98	3.54	46	0.434	0.077	82%
MPB	0.98	0.02	5	0.196	0.004	98%
CBZ	0.35	0.31	2	0.173	0.154	11%
NPX	1.61	0.95	17	0.095	0.056	41%
DCF	0.36	0.34	5	0.073	0.067	8%
NOR	0.72	0.43	16	0.045	0.027	41%
CIP	2.51	0.58	89	0.028	0.007	77%
SMTX	0.05	0.01	6	0.008	0.002	69%
MTP	0.37	0.10	86	0.004	0.001	72%
SMRZ	0.29	0.08	68	0.004	0.001	72%
PPB	0.42	0.01	123	0.003	0.000	98%
TMP	0.37	0.04	120	0.003	0.000	89%
SMTZ	0.04	0.02	30	0.001	0.001	59%
PEF	0.73	0.66	257527	0.000	0.000	10%
ENR	0.44	0.20	160834	0.000	0.000	54%
OFL	1.48	0.46	1.39·10 ¹⁴	0.000	0.000	69%