

## **Supplementary Information to the article:**

### **Sorption and desorption of diverse contaminants of varying polarity in wastewater sludge with and without alum**

**Marie-France Morissette<sup>1</sup>, Sung Vo Duy<sup>1</sup>, Hans Peter H. Arp<sup>2</sup>, Sébastien Sauvé<sup>1\*</sup>**

<sup>1</sup>Department of Chemistry, Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montreal, QC, Canada H3C 3J7

<sup>2</sup> Norwegian Geotechnical Institute (NGI), P.O. Box 3930 Ullevål Stadion, N-0806 Oslo, Norway

\*Corresponding author:

Sébastien Sauvé, Ph.D.,  
Full Professor  
Université de Montréal  
Pavillon Roger-Gaudry, Chimie  
CP 6128 Centre-ville  
Montréal, QC, H3C 3J7  
Canada

Tel 514 343-6749 Fax 514 343-2468, e-mail: [sebastien.sauve@umontreal.ca](mailto:sebastien.sauve@umontreal.ca)

# **S1. Batch equilibrium sorption kinetic model background information**

According to the Organisation for Economic Co-operation and Development (OECD) guideline, kinetic sorption/desorption studies can be performed using a parallel or serial batch equilibrium method <sup>1</sup>. In the parallel method, several samples with the same liquid/solid ratios are prepared and one (or many) of the total number of samples are removed and analyzed at each selected time step. One drawback of this method is that samples are independent which may increase variability when dealing with a highly heterogeneous matrix such as wastewaters or sewage. In the serial method, a sample is prepared in duplicate. At each time step, a subsample is pipetted and centrifuged, an aliquot of the aqueous phase is taken and analyzed while the rest of the sample is resuspended and the experiment continues. Even if manipulations are more laborious with the parallel method, it is often preferred given its simpler mathematical treatment of results <sup>1</sup>.

## S2. Instrumental Conditions

**Table S1. Gradient elution conditions used for solid phase extraction and chromatographic separation**

Loading pump				Analytical pump			
Time (min)	A (%)	B (%)	Flow rate ( $\mu\text{L min}^{-1}$ )	Time (min)	A (%)	B (%)	Flow rate ( $\mu\text{L min}^{-1}$ )
On-line SPE loading				Column equilibration			
0.00	100	0	1500	0.00	60	40	525
0.92	100	0	1500	0.92	60	40	525
Loop wash then SPE column wash				Elution and chromatographic separation			
0.93	0	100	1500	2.45	45	55	525
4.50	0	100	1500	4.00	25	75	525
SPE column conditioning				5.10	20	80	525
4.51	100	0	1500	Column equilibration			
				5.11	60	40	525
				7.00	60	40	525

A : H<sub>2</sub>O + 0.1 % HCOOH

B : MeOH + 0.1 % HCOOH

**Table S2. MS/MS optimized parameters for all selected compounds**

Compound	Precursor ion (m/z)	Product ion (m/z)	Intensity ratio (%)	TL (V)	CE (eV)
CAF	195	138	100	80	19
	[M+H]	110	14 ± 1	80	23
SMX	254	92	100	71	28
	[M+H] <sup>+</sup>	108	77 ± 3	71	25
DEA	188	146	100	74	18
	[M+H] <sup>+</sup>	104	16 ± 1	74	22
CBZ	237	194	100	77	18
	[M+H] <sup>+</sup>	192	26 ± 1	77	23
ATZ	216	174	100	71	18
	[M+H] <sup>+</sup>	104	16 ± 1	71	31
E2	255	159	100	100	17
	[M-H <sub>2</sub> O+H] <sup>+</sup>	133	37 ± 1	100	16
EE2	279	133	100	87	15
	[M-H <sub>2</sub> O+H] <sup>+</sup>	159	86 ± 4	87	18
NOR	299	109	100	114	37
	[M-H <sub>2</sub> O+H] <sup>+</sup>	91	59 ± 4	114	22
DCF	296	250	100	73	18
	[M+H] <sup>+</sup>	215	85 ± 7	73	14
CAF*	198	140	-	81	18
SMX*	260	98	-	77	27
CBZ*	247	204	-	82	20
ATZ*	219	177	-	84	17
E2*	261	159	-	83	29
DCF*	300	219	-	70	19

## S3. Analytical Validation and Quality Assurance / Quality Control

**Table S3.** Validation parameters including correlation coefficient, LOD, LOQ and linearity of the method in filtered tap water and wastewater

Compound	Tap water				Wastewater			
	R <sup>2</sup>	LOD (ng/L)	LOQ (ng/L)	Linearity (ng/L)	R <sup>2</sup>	LOD (ng/L)	LOQ (ng/L)	Linearity (ng/L)
CAF	1.0000	0.5	1.5	1.5-50000	0.9979	115	345	345-50000
SMX	0.9998	1.0	3.0	3.0-50000	0.9993	30	90	90-50000
DEA	0.9996	1.0	3.0	3.0-50000	0.9993	35	105	105-50000
CBZ	0.9983	1.0	3.0	3.0-50000	0.9985	65	195	195-50000
ATZ	0.9995	0.5	1.5	1.5-50000	0.9983	25	75	75-50000
E2	0.9994	5.0	15.0	15.0-50000	0.9989	115	345	345-50000
EE2	0.9991	5.0	15.0	15.0-50000	0.9976	110	330	330-50000
NOR	0.9995	20.0	60.0	60.0-50000	0.9998	100	300	300-50000
DCF	0.9992	5.0	15.0	15.0-50000	0.9989	15	45	45-50000

**Table S4.** Validation parameters including repeatability (intra-day, n= 5) and reproductibility (inter-day, n =3) of the method in filtered tap water and wastewater

Compound	Tap water				Wastewater			
	Repeat. 300 ng/L (%)	Reprod. 300 ng/L (%)	Repeat. 10000 ng/L (%)	Reprod. 10000 ng/L (%)	Repeat. 300 ng/L (%)	Reprod. 300 ng/L (%)	Repeat. 10000 ng/L (%)	Reprod. 10000 ng/L (%)
CAF	3	4	2	3	2	3	2	3
SMX	4	7	2	3	8	6	5	3
DEA	3	8	2	6	5	7	2	3
CBZ	5	6	6	8	2	5	5	5
ATZ	3	8	2	3	2	4	2	5
E2	6	10	3	7	5	10	5	5
EE2	6	10	6	8	5	13	6	10
NOR	5	9	2	6	9	12	4	15
DCF	7	9	4	7	5	9	4	7

## S4. Recoveries and Mass Balance

**Table S5.** Extraction recoveries (mean  $\pm$  SD) of each compound in sludge particles (n=3)

Compound	Recoveries (%)	
	50 ng g <sup>-1</sup>	200 ng g <sup>-1</sup>
CAF*	72 $\pm$ 2	60 $\pm$ 3
SMX	60 $\pm$ 9	59 $\pm$ 5
DEA	97 $\pm$ 1	95 $\pm$ 5
CBZ	99 $\pm$ 10	97 $\pm$ 9
ATZ	94 $\pm$ 4	95 $\pm$ 5
E2	60 $\pm$ 12	61 $\pm$ 3
EE2	103 $\pm$ 12	94 $\pm$ 3
NOR	96 $\pm$ 2	96 $\pm$ 12
DCF	60 $\pm$ 10	86 $\pm$ 9

\* spiked at 500 and 2000 ng g<sup>-1</sup>

**Table S6.** Mass balance average from each sorption and desorption experiment

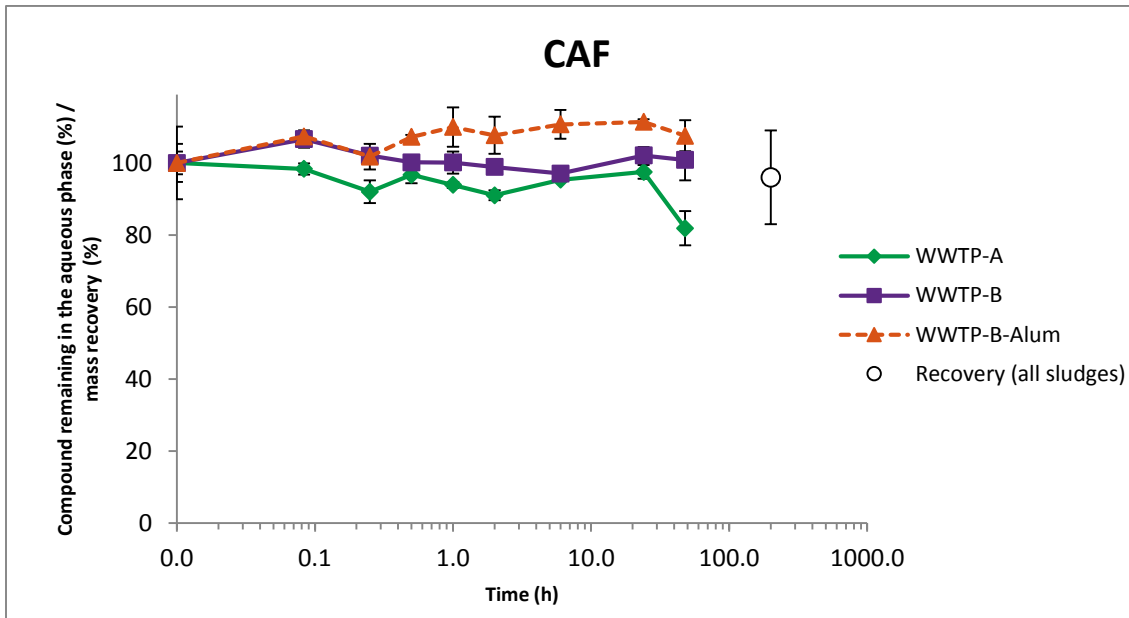
Compound	Sorption Mean $\pm$ SD (%)	Desorption Mean $\pm$ SD (%)
CAF	96 $\pm$ 13	91 $\pm$ 2
SMX	25 $\pm$ 45	82 $\pm$ 13
DEA	77 $\pm$ 28	103 $\pm$ 11
CBZ	100 $\pm$ 9	90 $\pm$ 11
ATZ	77 $\pm$ 31	77 $\pm$ 19
E2	21 $\pm$ 8	7 $\pm$ 7
EE2	51 $\pm$ 19	44 $\pm$ 2
NOR	18 $\pm$ 32	63 $\pm$ 15
DCF	69 $\pm$ 18	57 $\pm$ 15

**Table S7.** Compound remaining in aqueous phase after 5 min and 48 h in the three different sludge samples

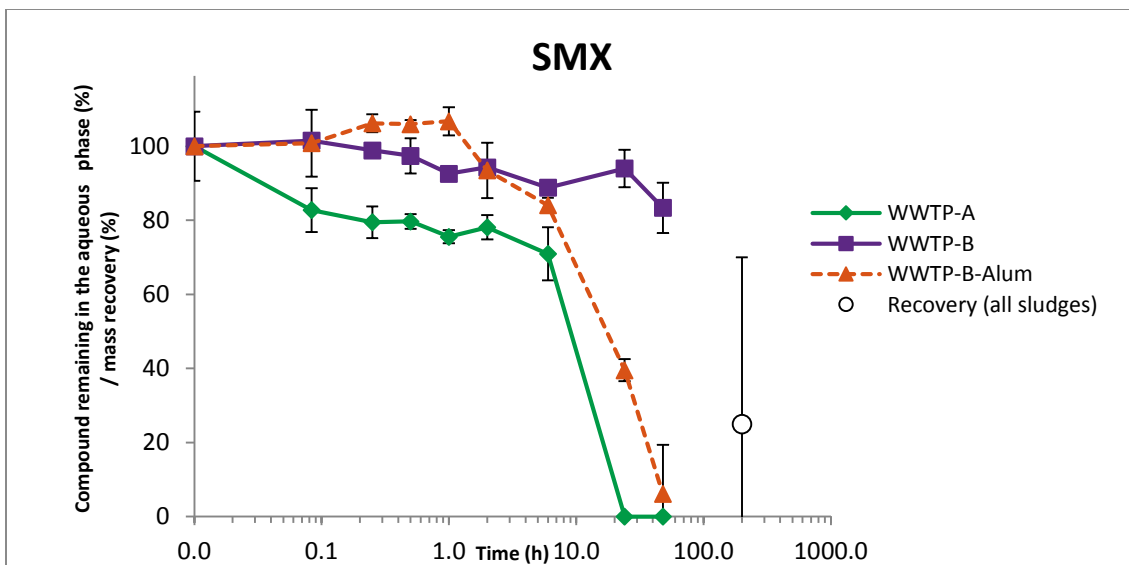
Compound	WWTP-A (%)		WWTP-B (%)		WWTP-B-Alum (%)	
	5 min	48 h	5 min	48 h	5 min	48 h
CAF	98	82	107	101	107	108
SMX	83	0	102	83	101	6
DEA	99	29	103	87	105	97
CBZ	79	78	96	90	99	90
ATZ	54	36	102	88	98	91
E2	20	10	40	7	70	26
EE2	10	14	23	19	43	36
NOR	34	0	61	42	83	0
DCF	39	48	46	35	98	87

# S5. Aqueous Concentration Changes After Spiking (Sorption Experiment)

Data from the sorption kinetics experiment is presented in Figures S1-9 and Tables S8-16.

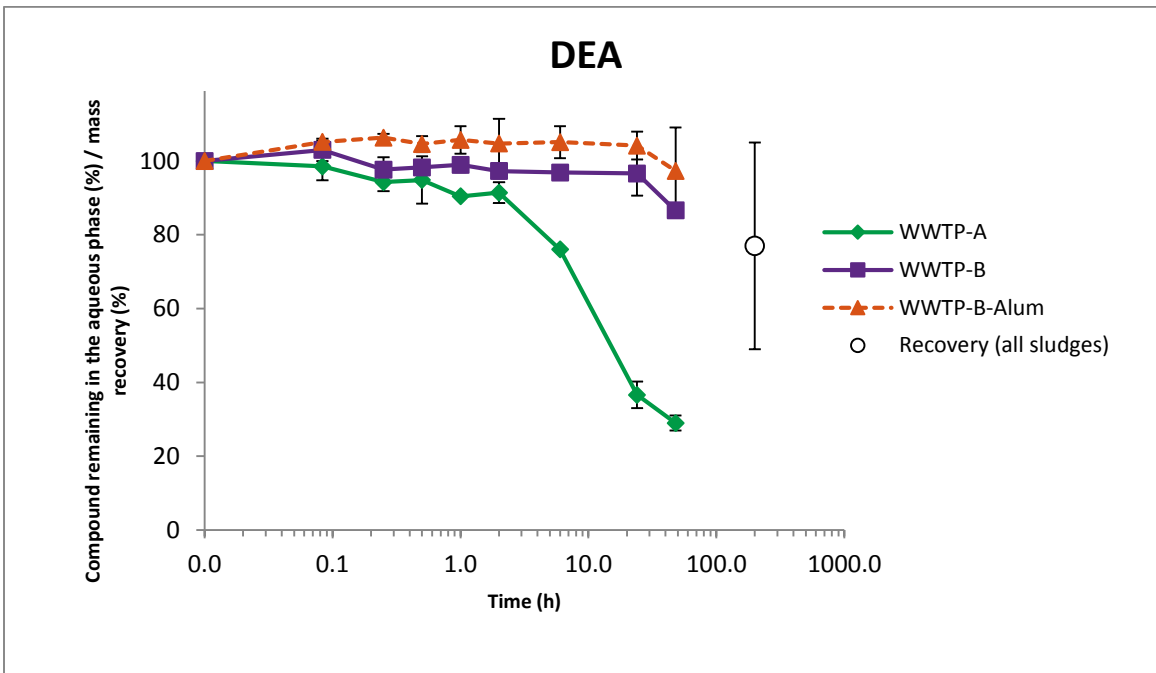


**Figure S1.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for caffeine in the three different sludge samples

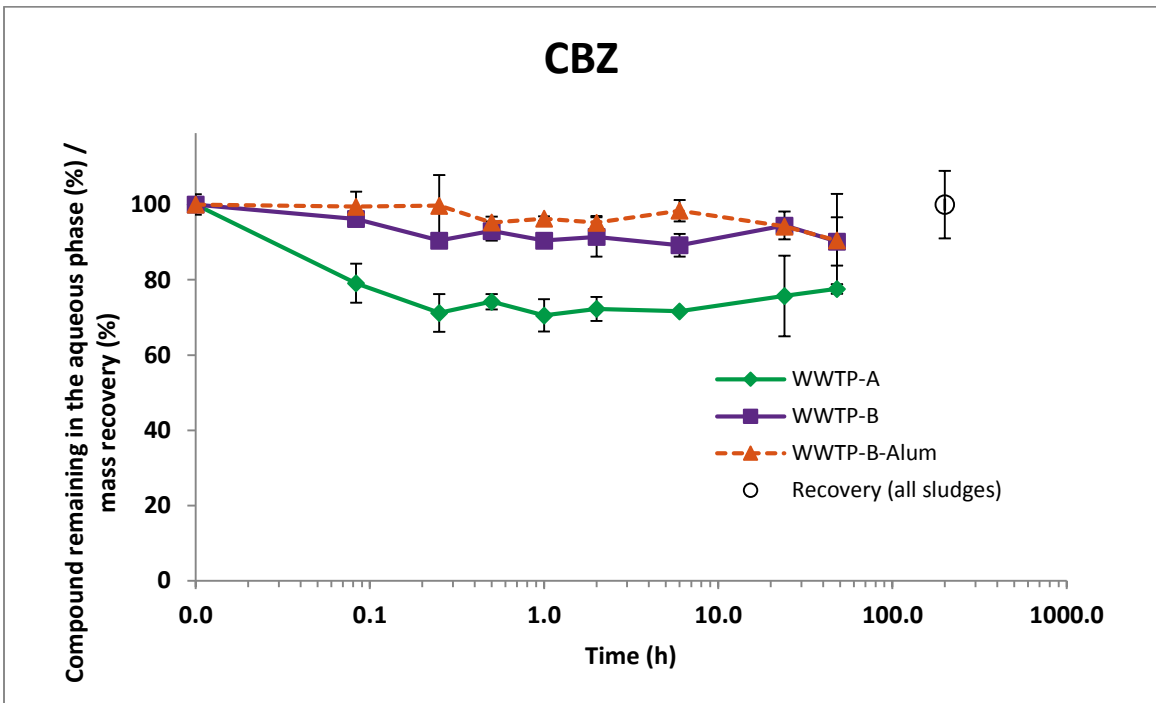


**Figure S2.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for sulfamethoxazole in the three different sludge samples

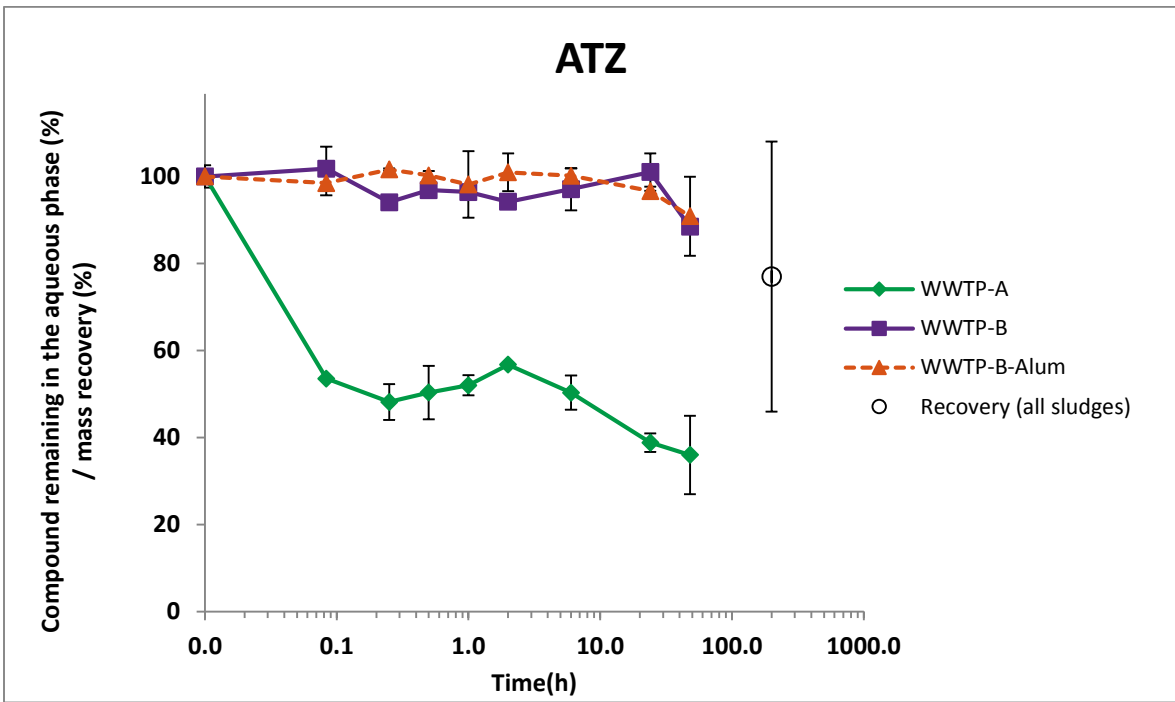




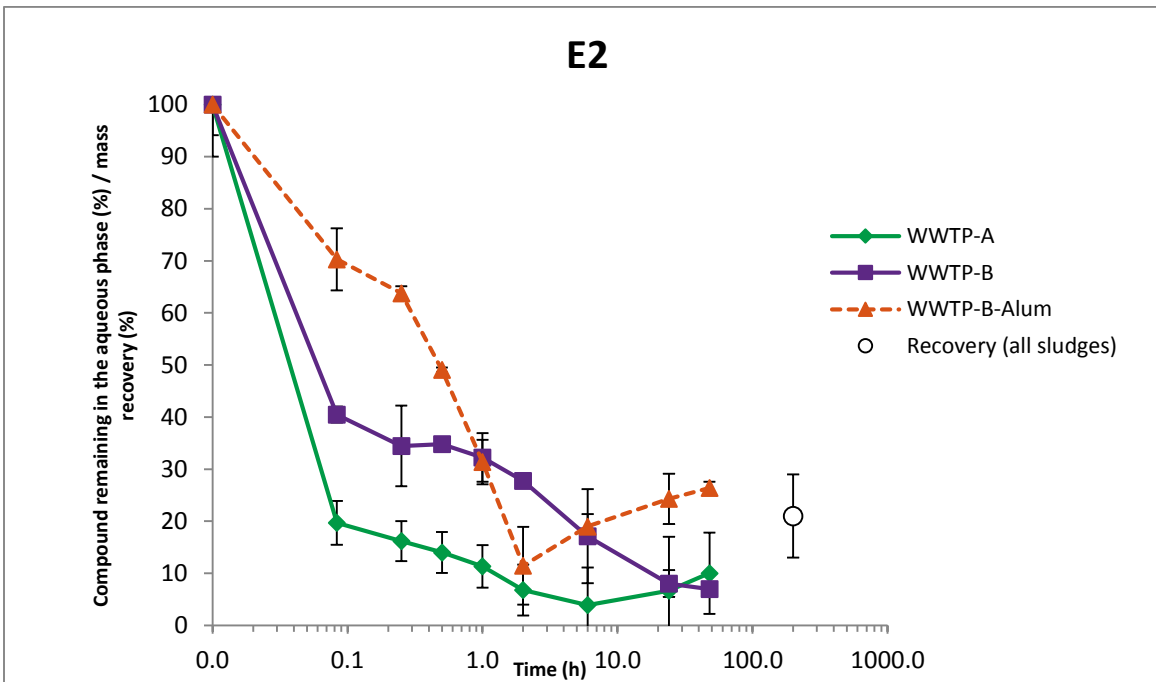
**Figure S3.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for desethylatrazine in the three different sludge samples.



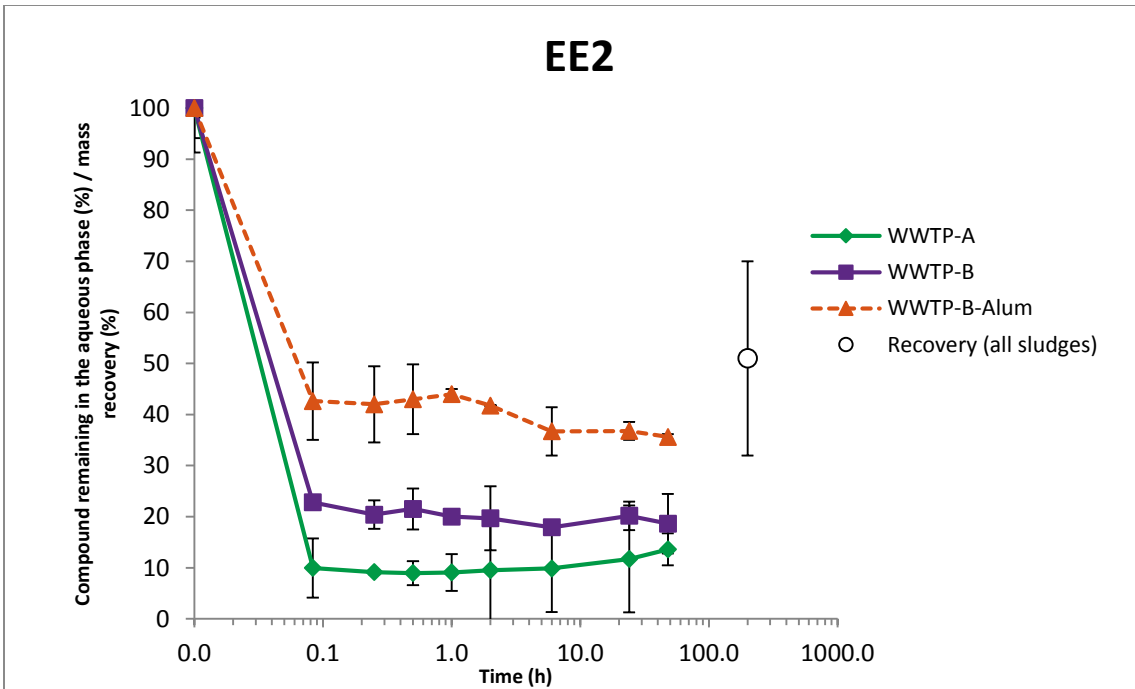
**Figure S4.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for carbamazepine in the three different sludge samples.



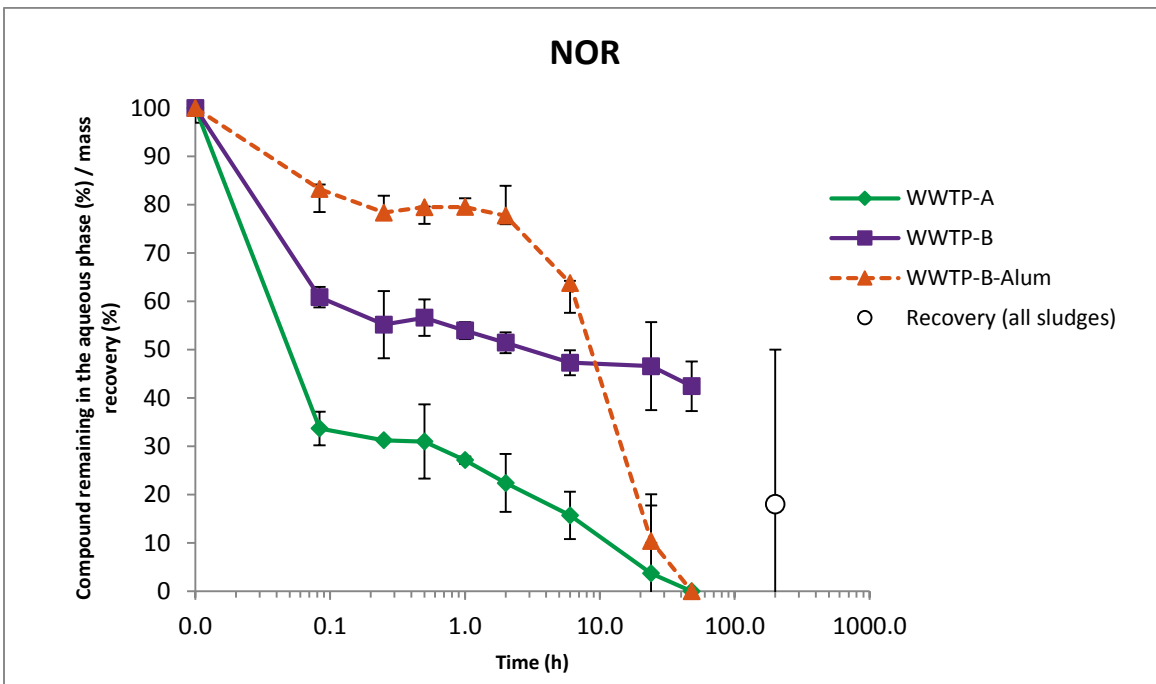
**Figure S5.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for atrazine in the three different sludge samples.



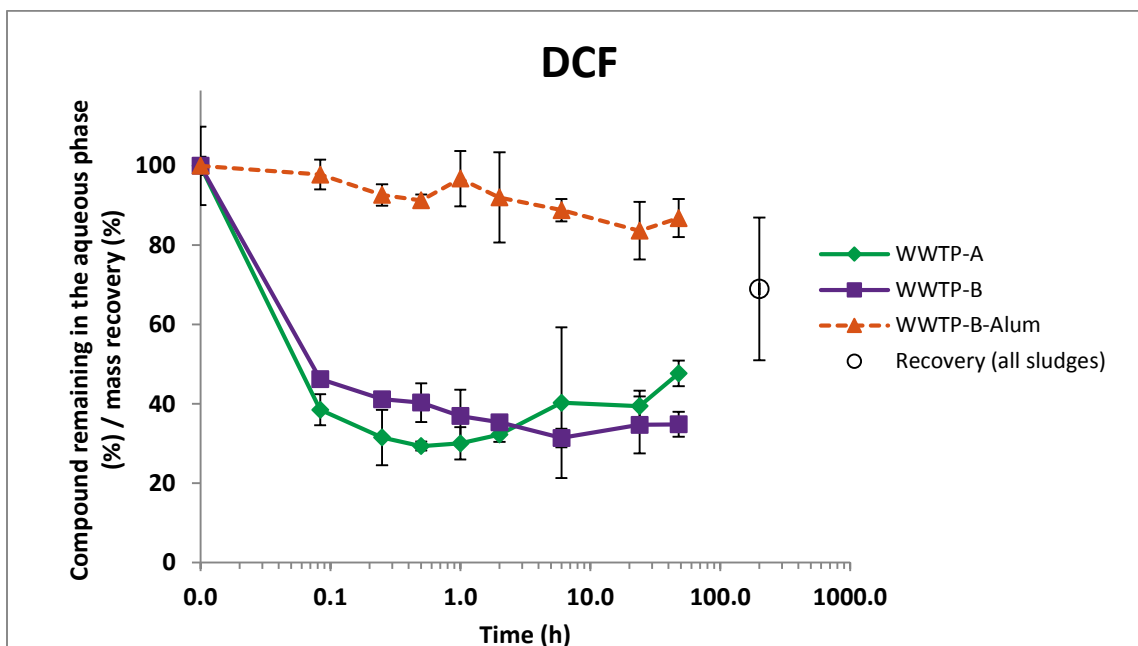
**Figure S6.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for 17β-estradiol in the three different sludge samples



**Figure S7.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for ethinylestradiol in the three different sludge samples



**Figure S8.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for norethindrone in the three different sludge samples



**Figure S9.** Aqueous phase concentration remaining vs time shaken after spiking and mass recovery for diclofenac in the three different sludge samples

**Table S8.** Aqueous phase concentration of caffeine vs time shaken after spiking

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	50.7	100.0	10.1	51.5	100.0	3.1	76.1	100.0	5.3
0.08	49.8	98.3	1.6	54.9	106.6	2.4	81.4	107.4	1.6
0.25	46.6	92.0	3.2	52.6	102.0	1.5	77.4	101.7	3.5
0.5	49.0	96.7	2.3	51.6	100.2	0.6	81.3	107.2	0.6
1	47.6	93.9	0.8	51.6	100.1	3.1	83.3	110.0	5.4
2	46.1	91.0	1.4	50.9	98.9	0.8	81.7	107.7	5.1
6	48.3	95.3	0.2	50.0	97.1	1.2	83.8	110.7	4.0
24	49.4	97.5	1.9	52.6	102.1	2.3	84.3	111.4	0.7
48	41.5	81.9	4.7	51.9	100.8	5.6	81.6	107.6	4.3

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S9. Aqueous phase concentration of sulfamethoxazole vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	23.4	100.0	9.3	20.7	100.0	0.8	18.6	100.0	0.2
0.08	19.4	82.8	5.9	21.028	101.5	1.8	18.754	100.8	9.0
0.25	18.6	79.5	4.3	20.5	98.9	0.9	19.8	106.2	2.4
0.5	18.7	79.7	2.0	20.2	97.4	4.8	19.7	106.0	1.1
1	17.7	75.6	1.8	19.2	92.6	0.1	19.9	106.7	3.8
2	18.3	78.1	3.3	19.5	94.3	1.5	17.4	93.5	7.5
6	16.6	70.9	7.2	18.4	88.8	0.2	15.6	84.1	2.0
24	< LOD	-	-	19.5	94.0	5.1	7.4	39.5	3.0
48	< LOD	-	-	17.3	83.4	6.8	1.1	6.1	13.2

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S10. Aqueous phase concentration of desethylatrazine vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	19.9	100.0	-	22.3	100.0	1.4	20.0	100.0	1.3
0.08	19.6	98.5	3.7	22.9	103.0	3.0	21.1	105.2	0.3
0.25	18.8	94.3	2.4	21.7	97.7	3.4	21.3	106.3	1.0
0.5	18.9	94.8	6.4	21.9	98.2	0.6	20.9	104.6	2.2
1	18.0	90.4	0.3	22.0	98.9	2.0	21.2	105.7	3.7
2	18.2	91.4	2.8	21.7	97.3	1.9	21.0	104.7	6.7
6	15.1	76.0	0.4	21.6	96.9	1.5	21.0	105.1	4.3
24	7.3	36.6	3.6	21.5	96.6	6.0	20.9	104.2	3.7
48	5.8	29.0	2.0	19.3	86.6	1.2	19.5	97.3	11.7

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S11. Aqueous phase concentration of carbamazepine vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	21.7	100.0	0.1	34.5	100.0	0.0	18.9	100.0	2.7
0.08	17.1	79.1	5.2	33.165	96.2	1.0	18.784	99.5	4.0
0.25	15.4	71.2	5.0	31.2	90.4	0.7	18.8	99.7	8.2
0.5	16.1	74.2	2.0	32.1	93.0	2.5	18.0	95.3	1.5
1	15.3	70.5	4.3	31.2	90.4	1.0	18.2	96.3	0.6
2	15.6	72.3	3.2	31.5	91.4	5.2	18.0	95.2	1.8
6	15.5	71.7	0.3	30.8	89.2	3.1	18.6	98.4	2.9
24	16.4	75.7	10.7	32.6	94.5	3.7	17.8	94.2	0.7
48	16.8	77.6	1.3	31.1	90.2	6.4	17.1	90.5	12.4

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S12. Aqueous phase concentration of atrazine vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	20.9	100.0	-	20.1	100.0	0.0	19.2	100.0	2.6
0.08	11.2	53.5	0.2	20.4	101.8	5.0	18.9	98.5	2.8
0.25	10.1	48.2	4.1	18.9	94.1	1.7	19.5	101.6	0.2
0.5	10.5	50.4	6.1	19.5	96.9	1.8	19.2	100.2	1.0
1	10.9	52.0	2.3	19.4	96.4	0.1	18.8	98.2	7.7
2	11.9	56.8	0.4	18.9	94.2	0.0	19.4	101.0	4.4
6	10.5	50.3	3.9	19.5	97.1	4.9	19.2	100.2	1.7
24	8.1	38.8	2.2	20.3	101.0	4.3	18.5	96.6	1.0
48	7.5	36.0	9.0	17.8	88.5	1.6	17.4	90.9	9.1

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S13. Aqueous phase concentration of 17 $\beta$ -estradiol vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase ( $\mu\text{g/L}$ )	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase ( $\mu\text{g/L}$ )	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase ( $\mu\text{g/L}$ )	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	19.3	100.0	5.9	16.6	100.0	1.3	16.8	100.0	10.0
0.08	3.8	19.7	4.2	6.7	40.5	1.6	11.8	70.3	6.0
0.25	3.1	16.2	3.8	5.7	34.5	7.7	10.7	63.8	1.3
0.5	2.7	14.0	3.9	5.8	34.8	0.4	8.3	49.1	0.4
1	2.2	11.3	4.1	5.3	32.2	4.7	5.3	31.4	4.3
2	1.3	6.8	4.9	4.6	27.7	0.9	1.9	11.5	7.4
6	0.8	3.9	7.2	2.8	17.1	9.0	3.2	19.0	2.4
24	1.3	6.7	10.3	1.3	8.0	2.6	4.1	24.3	4.8
48	1.9	10.0	7.8	1.2	7.0	0.0	4.4	26.4	1.2

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S14. Aqueous phase concentration of ethinylestradiol vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase ( $\mu\text{g/L}$ )	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase ( $\mu\text{g/L}$ )	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase ( $\mu\text{g/L}$ )	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	19.7	100.0	1.9	19.1	100.0	5.9	19.5	100.0	8.7
0.08	2.0	10.0	5.8	4.362	22.8	1.4	8.3	42.6	7.6
0.25	1.8	9.2	0.4	3.9	20.4	2.8	8.2	42.0	7.4
0.5	1.8	9.0	2.3	4.1	21.5	4.0	8.4	43.0	6.8
1	1.8	9.1	3.6	3.8	20.0	0.2	8.6	44.0	1.0
2	1.9	9.5	11.4	3.8	19.7	6.3	8.2	41.8	0.1
6	1.9	9.9	8.6	3.4	17.9	1.0	7.2	36.7	4.7
24	2.3	11.7	10.5	3.9	20.2	2.8	7.2	36.8	1.7
48	2.7	13.6	3.1	3.6	18.6	5.8	7.0	35.6	0.5

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S15. Aqueous phase concentration of norethindrone vs time shaken after spiking**

Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	20.2	100.0	-	22.8	100.0	3.0	19.8	100.0	4.7
0.08	6.8	33.7	3.5	13.907	60.9	2.1	16.473	83.2	1.0
0.25	6.3	31.3	0.1	12.6	55.2	7.0	15.5	78.4	3.5
0.5	6.3	31.0	7.7	12.9	56.6	3.8	15.7	79.5	0.1
1	5.5	27.1	0.8	12.3	54.0	1.7	15.7	79.5	1.8
2	4.5	22.4	6.0	11.8	51.5	2.2	15.4	77.7	6.2
6	3.2	15.7	4.9	10.8	47.3	2.6	12.6	63.8	0.4
24	0.8	3.7	14.0	10.6	46.6	9.1	2.1	10.4	9.6
48	< LOD	-	-	9.7	42.4	5.1	< LOD	-	-

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

**Table S16. Aqueous phase concentration of diclofenac vs time shaken after spiking**

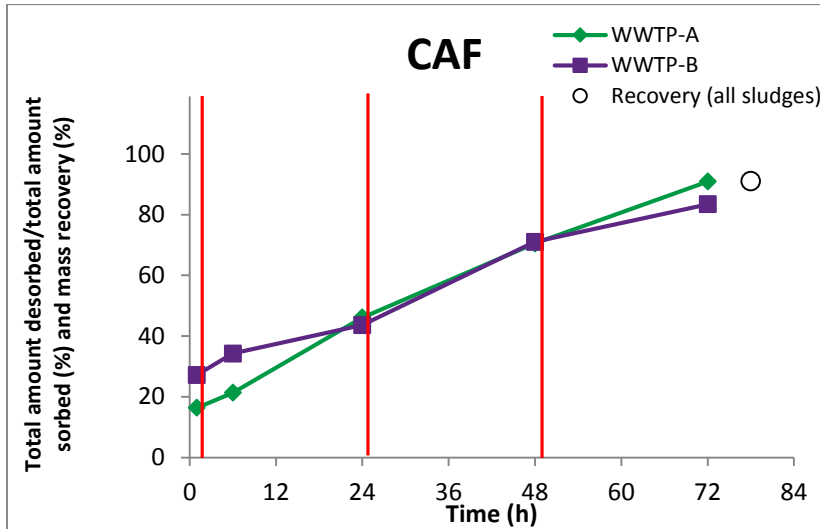
Time shaken (h)	WWTP-A			WWTP-B			WWTP-B Alum		
	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD	Concentration in the aqueous phase (µg/L)	Normalized concentration relative to the initial concentration* (%)	SD
0.01*	12.3	100.0	9.8	17.4	100.0	2.3	18.1	100.0	0.9
0.08	4.7	38.5	3.9	8.0	46.3	0.8	17.7	97.9	3.7
0.25	3.9	31.5	7.0	7.2	41.2	0.2	16.8	92.8	2.6
0.5	3.6	29.4	1.1	7.0	40.3	4.9	16.6	91.5	1.5
1	3.7	30.1	4.1	6.4	37.0	6.6	17.6	96.9	6.8
2	4.0	32.3	1.8	6.2	35.4	0.6	16.7	92.2	11.2
6	5.0	40.3	19.0	5.5	31.4	2.3	16.1	89.0	2.8
24	4.9	39.5	3.9	6.0	34.7	7.2	15.2	83.9	7.1
48	5.9	47.7	3.2	6.1	34.9	3.1	15.8	87.1	4.7

\* Concentration at T=0 was determined to be the concentration remaining in the aqueous phase in the control sample after 48h of shaking

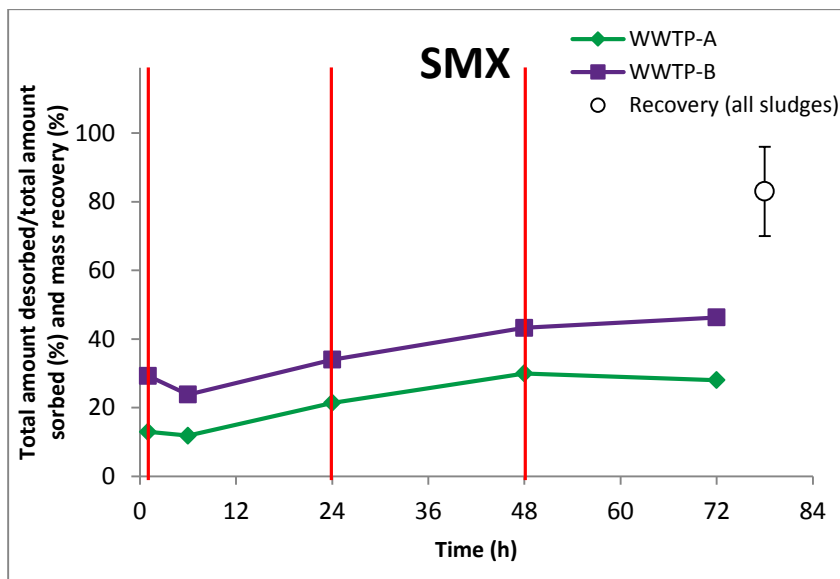


# S6. Desorption and Rinsing Figures

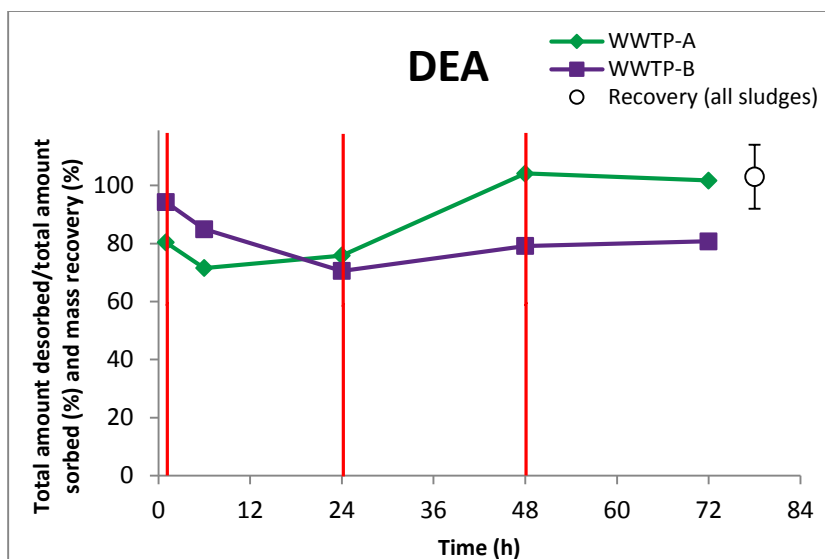
Data from the desorption kinetics experiment is presented in Figures S10-18 and Tables S17-25.



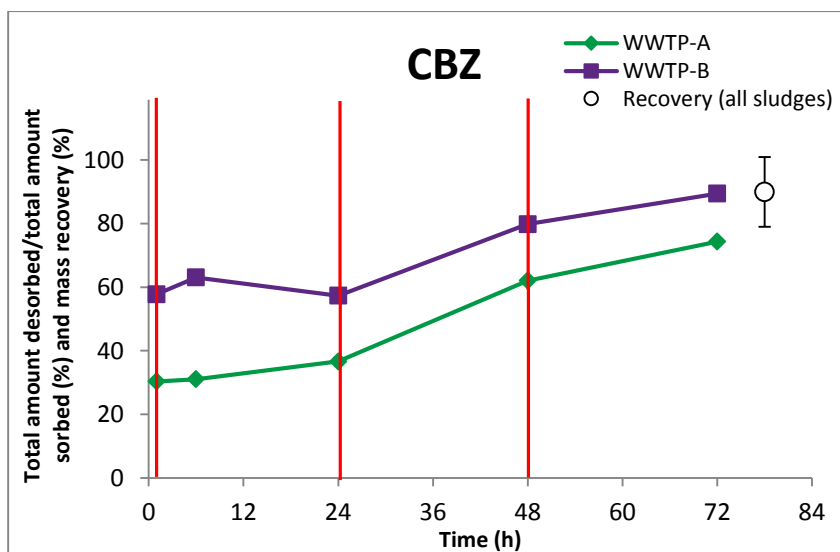
**Figure S10.** Cumulative desorption of caffeine in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



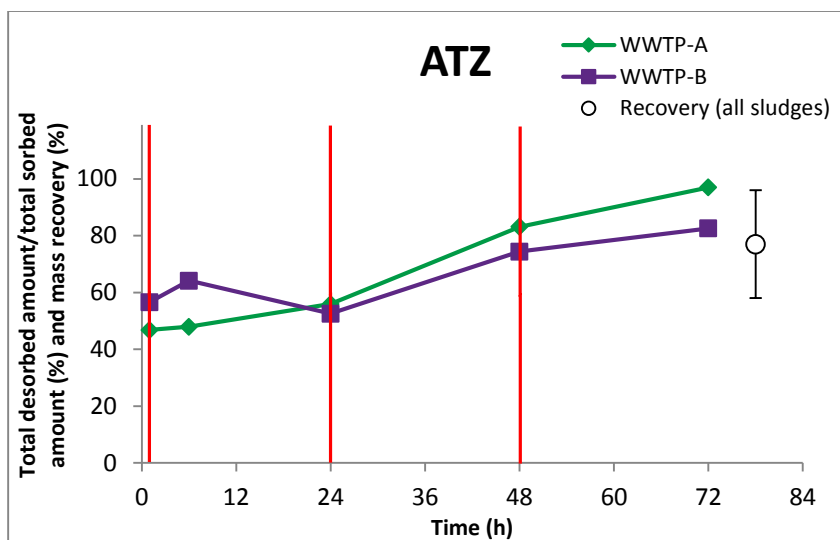
**Figure S11.** Cumulative desorption of sulfamethoxazole in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



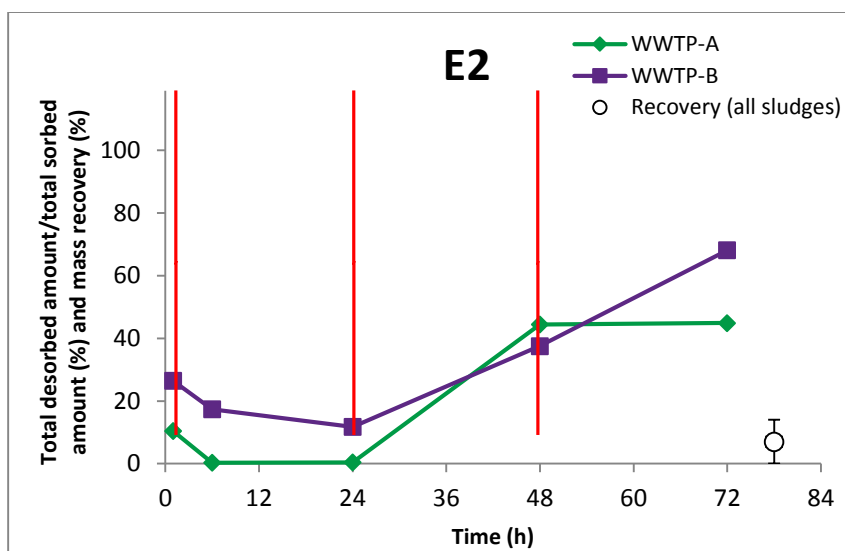
**Figure S12.** Cumulative desorption of desethylatrazine in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



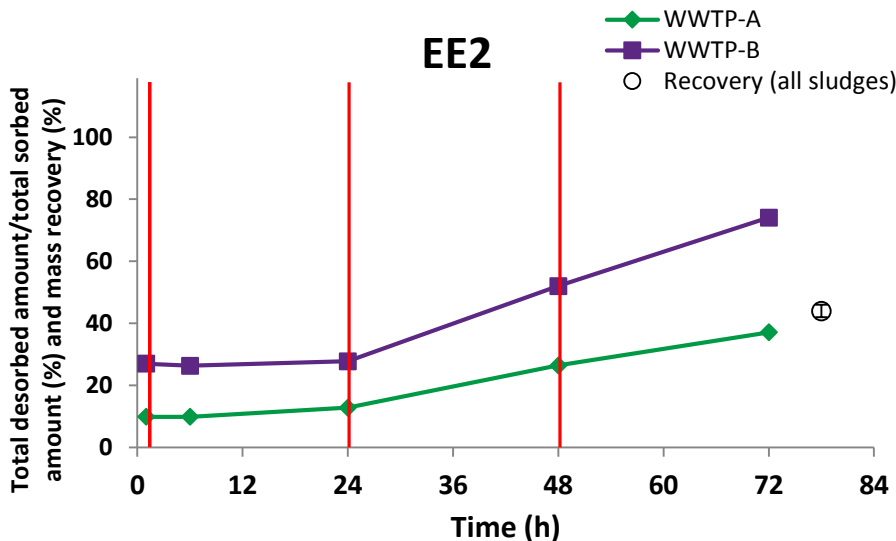
**Figure S13.** Cumulative desorption of carbamazepine in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



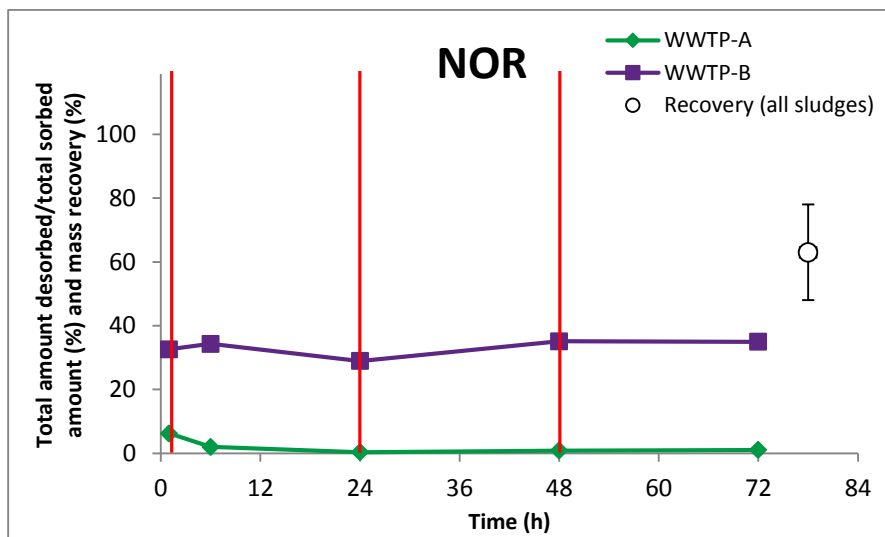
**Figure S14.** Cumulative desorption of atrazine in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



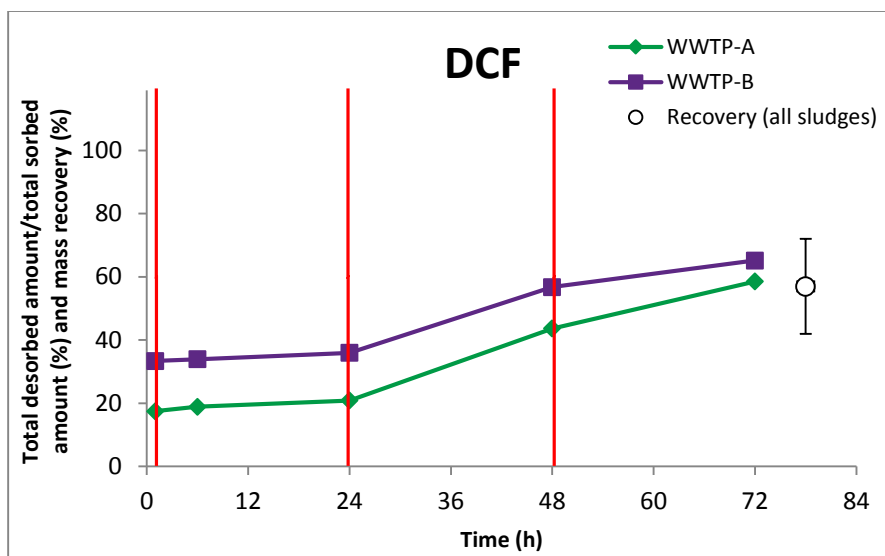
**Figure S15.** Cumulative desorption of 17 $\beta$ -estradiol in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



**Figure S16.** Cumulative desorption of ethinylestradiol in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



**Figure S17.** Cumulative desorption of norethindrone in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.



**Figure S18.** Cumulative desorption of diclofenac in the two different sludge samples as a function of time and rinsing step (indicated by vertical lines) relative to the amount sorbed and mass recovery compared to the original spiked amount.

**Table S17.** Released concentration of caffeine from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	81.2	16.4	209.9	27.2
[1-6h]	24.5	21.3	54.5	34.2
[6-24h]	122.7	46.1	72.6	43.6
[24-48h]	120.9	70.5	211.7	71.0
[48-72h]	101.0	90.9	95.9	83.4

\* For compound with mass balance < 80 % after sorption, the mass balance was taken into account in the expected desorbed concentration considering that what was lost could not desorb from the solid phase (i.e. Cumulative desorbed = (amount in aqueous phase)/(mass sorbed to solid phase after sorption experiment)).

**Table S18.** Released concentration of sulfamethoxazole from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	22.5	13.0	78.9	29.3
[1-6h]	-1.9	11.9	-14.8	23.8
[6-24h]	16.5	21.4	27.4	34.0
[24-48h]	14.8	30.0	25.0	43.3
[48-72h]	-3.4	28.0	8.2	46.3

\* For compound with mass balance < 80 % after sorption, the mass balance was taken into account in the expected desorbed concentration considering that what was lost could not desorb from the solid phase (i.e. Cumulative desorbed = (amount in aqueous phase)/(mass sorbed to solid phase after sorption experiment)).

**Table S19.** Released concentration of desethylatrazine from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	346	80.4	405.4	94.2
[1-6h]	-38	71.6	-39.9	85.0
[6-24h]	18	75.8	-62.0	70.5
[24-48h]	100	104.1	37.0	79.1
[48-72h]	-10	101.7	7.1	80.8

**Table S20.** Released concentration of carbamazepine from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	158.7	30.3	389.9	57.8
[1-6h]	3.8	31.1	35.6	63.1
[6-24h]	29.2	36.6	-38.9	57.3
[24-48h]	133.1	62.1	151.9	79.8
[48-72h]	64.2	74.3	65.0	89.5

\* For compound with mass balance < 80 % after sorption, the mass balance was taken into account in the expected desorbed concentration considering that what was lost could not desorb from the solid phase (i.e. Cumulative desorbed = (amount in aqueous phase)/(mass sorbed to solid phase after sorption experiment).

**Table S21.** Released concentration of atrazine from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	197.0	46.8	415.2	56.6
[1-6h]	4.8	47.9	55.6	64.2
[6-24h]	33.7	55.9	-85.1	52.6
[24-48h]	114.7	83.2	160.4	74.4
[48-72h]	58.2	97.0	59.9	82.6

\* For compound with mass balance < 80 % after sorption, the mass balance was taken into account in the expected desorbed concentration considering that what was lost could not desorb from the solid phase (i.e. Cumulative desorbed = (amount in aqueous phase)/(mass sorbed to solid phase after sorption experiment).

**Table S22.** Released concentration of 17 $\beta$ -estradiol from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	3.9	10.4	81.6	26.5
[1-6h]	-3.7	0.3	-28.0	17.4
[6-24h]	0.0	0.4	-17.4	11.7
[24-48h]	16.3	44.4	79.6	37.5
[48-72h]	0.2	44.9	94.4	68.1

**Table S23.** Released concentration of ethinylestradiol from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	60.5	9.9	247.8	27.0
[1-6h]	-0.1	9.9	-5.9	26.4
[6-24h]	18.1	12.9	13.2	27.8
[24-48h]	82.9	26.4	222.6	52.1
[48-72h]	65.1	37.1	202.5	74.1

\* For compound with mass balance < 80 % after sorption, the mass balance was taken into account in the expected desorbed concentration considering that what was lost could not desorb from the solid phase (i.e. Cumulative desorbed = (amount in aqueous phase)/(mass sorbed to solid phase after sorption experiment).

**Table S24.** Released concentration of norethindrone from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	45.0	6.2	361.6	32.6
[1-6h]	-30.3	2.0	18.9	34.3
[6-24h]	-12.0	0.4	-59.3	29.0
[24-48h]	3.6	0.9	68.5	35.1
[48-72h]	1.3	1.1	-1.7	35.0

\* For compound with mass balance < 80 % after sorption, the mass balance was taken into account in the expected desorbed concentration considering that what was lost could not desorb from the solid phase (i.e. Cumulative desorbed = (amount in aqueous phase)/(mass sorbed to solid phase after sorption experiment).

**Table S25.** Released concentration of diclofenac from the solid phase of vs time

Time (h)	WWTP-A		WWTP-B	
	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)	Concentration desorbed (ng/g)	Cumulative normalized desorbed concentration relative to the expected desorbed concentration* (%)
[0-1h]	125.7	17.5	526.8	33.4
[1-6h]	10.4	18.9	8.6	33.9
[6-24h]	14.1	20.9	32.5	36.0
[24-48h]	164.2	43.7	328.4	56.8
[48-72h]	106.9	58.5	132.0	65.2



## S7. Rinsing factors and desorption $K_d$

Based on how the desorption work was done (multiple rinsing at fixed time steps), the determination of a desorption constant could not be derived using standard kinetic models. It was then decided to estimate rinsing factors, i.e., the number of rinsing steps needed to desorb 50 and 99 % of each compound, taking into account the desorbed quantities during the first three rinsings to a L/S value of 0.02 – 0.04 L/g<sub>dry sludge</sub>, using the equation:

$$\% \text{ desorbed} = m \ln(V_{\text{water}}) + b \quad (1)$$

Where  $V_{\text{water}}$  is the water needed to achieve a certain level of desorption, and  $m$  and  $b$  are regression coefficients. The number of rinsing steps required is then derived based on the extrapolated  $V_{\text{water}}$  needed, taking into account the volume used in each rinsing step (7 mL for WWTP-A and 8 mL for WWTP-B). Results are presented in Table S26. As expected, compounds with modest sorption would require fewer dilution steps (1 to 6) than compounds whose sorption is greater (2 to 53). Also, the data show that sludge samples coming from WWTP-A in which sorption was more pronounced (due to a higher OC content) would need more dilutions in order to fully desorb the compounds than the sludge samples from WWTP-B.

**Table S26.** Number of rinsing to L/S 0.02-0.04 needed for desorption in the two sludge samples

Compound	WWTP-A		WWTP-B	
	Number of rinsing (7 mL) needed for a desorption of		Number of rinsing (8 mL) needed for a desorption of	
	99%	50%	99%	50%
CAF	4	1	5	1
SMX	n.a.	n.a.	n.a.	n.a.
DEA	2	1	n.a.	n.a.
CBZ	6	2	2	1
ATZ	4	1	5	1
E2	n.a.	n.a.	n.a.	n.a.
EE2	53	6	6	2
NOR	n.a.	n.a.	n.a.	n.a.
DCF	10	3	10	2

n.a. = not applicable due to low mass balance and rapid transformation kinetics causing misleading results when used in equation 3.

**Table S27.** Solid water distribution coefficients of selected compounds in WWTP-A and WWTP-B samples with depletion in the samples as a function of rinsing step and time

Compound	WWTP-A (log $K_d$ )					WWTP-B (log $K_d$ )				
	Sor.	Des. 24 h	Des. 48h	Des. 72 h	Trend	Sor.	Des. 24 h	Des. 48h	Des. 72 h	Trend
CAF	0.8	1	1.1	0.9	≈	0.9	1.3	1.4	1.6	↑
SMX	0.8	1.1	1.5	2.1	↑	-0.1	1.2	1.8	2.4	↑
DEA	1.0	0.7	-0.5	0.7	≈	1.0	0.9	1.4	2	↑
CBZ	1.4	1.3	1.3	1.4	≈	0.5	1.2	1.3	1.4	↑
ATZ	-0.3	1.1	0.9	0.4	≈	0.1	1.4	1.5	1.7	↑
E2	2.1	2.3	1.5	2	≈	1.9	2.3	2	1.6	↓
EE2	2.4	2.1	2	2	≈	2.3	1.9	1.9	1.6	↓
NOR	1.8	2.9	3.3	3.6	↑	1.6	1.8	2.3	3.1	↑
DCF	1.7	2.8	3	3.2	↑	1.8	1.8	1.8	2.1	↑

## S8. Literature Review of Sludge $K_d$ and $K_{oc}$ values

**Table S28.** Literature review of  $K_d$  and  $K_{oc}$  previously reported

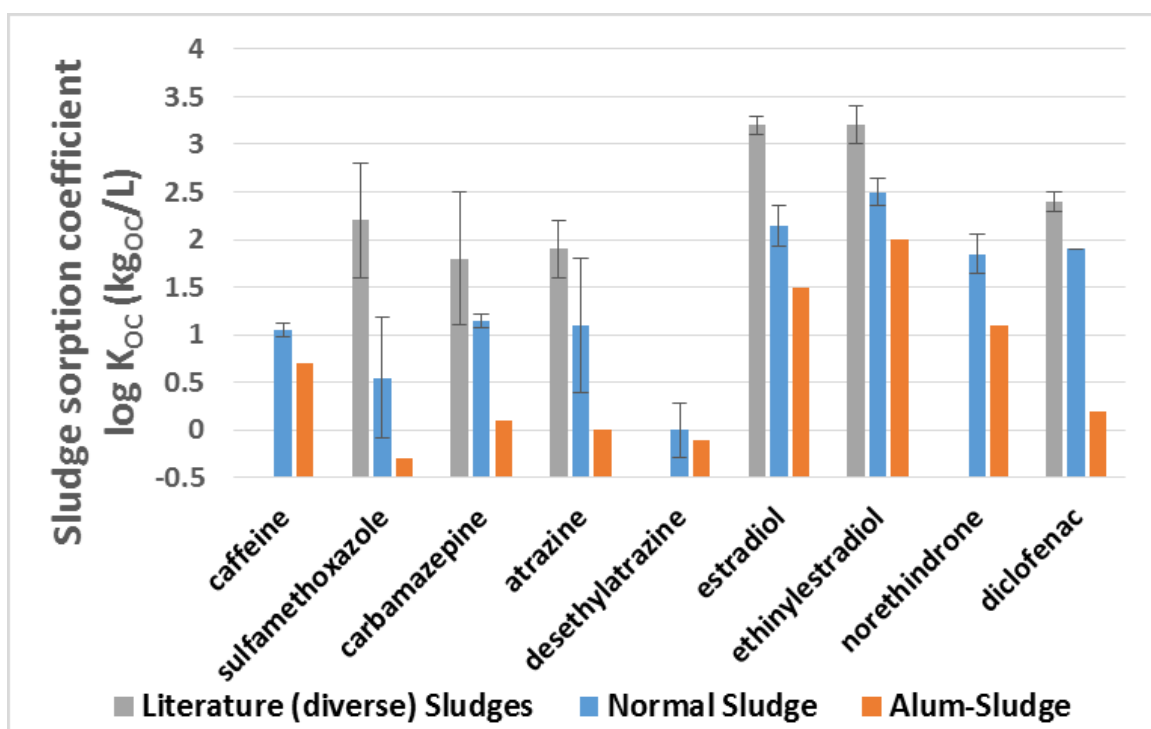
Compound	$K_D$ (L/kg) value (s.d.)	$K_{oc}$ (L/kg) value (s.d.)	Replicates	foc (%)	Sludge name / comments	Reference
ATZ		46 14				2
ATZ	100					3
ATZ	60 2	132				4
ATZ	122 24	245				4
ATZ	6	61		9.2 Ah		5
ATZ	7	68		9.9 Cg		5
ATZ	7	62		12 Cr		5
CAF	25				min thickened sludge, influenced by degradation?	6
CAF	100				max thickened sludge, influenced by degradation?	6
CAF	126				min digested sludge, influenced by degradation?	6
CAF	1259				max digested sludge, influenced by degradation?	6
CAF	32				cited in Narumiya etal	7
CAF	79				cited in Narumiya etal	7
CAF	<30				Denver Metro Activated Sludge	4
CAF	<30				Denver Metro Primary Sludge	4
CAF	<30				Mines Park Activated sludge	4
CAF	8				primary sludge	8
CAF	398				excess sludge (from figure 7 of reference)	8

Compound	K <sub>D</sub> (L/kg)		K <sub>OC</sub> (L/kg)		Replicates	f <sub>OC</sub> (%)	Sludge name / comments	Reference
	value	(s.d.)	value	(s.d.)				
CBZ	35		154			18 - 28	no pre-treatment	9
CBZ	63		363			11 - 23.8	alkaline	9
CBZ	40		174			19.6 -26.2	thermal	9
CBZ	56	11	193			29.2	ozone	9
CBZ	89	7	186		4	44.1		10
CBZ	237	79						11
CBZ	50						min thickened sludge	6
CBZ	100						max thickened sludge	6
CBZ	40						min digested sludge	6
CBZ	100						max digested sludge	6
CBZ	314	205			7		primary sludge	12
CBZ	135	39			7		second act.	12
CBZ	194	94			7		FS MBR	12
CBZ	164	49			7		HF MBR	12
CBZ	50	1	112					4
CBZ	65	5	129					4
CBZ	36	2	79					4
CBZ	1							13
CBZ	1	1	4	2	4-6		secondary sludge	14
CBZ	17	1	68	4		25		15
DCF	66	23	285			18 - 28	no pre-treatment	9
DCF	42	21	240			11 - 23.8	alkaline	9
DCF	37	12	161			19.6-26.2	thermal	9
DCF	151	16	347		6			10
DCF	200						min thickened sludge	6
DCF	1259						max thickened sludge	6
DCF	79						min digested sludge	6
DCF	158						max digested sludge	6
DCF	100						cited in Narumiya etal	7
DCF	316						cited in Narumiya etal	7
DCF	194	134			7		primary sludge	12
DCF	118	95			7		second act.	12
DCF	197	255			7		FS MBR	12
DCF	321	402			7		HF MBR	12
DCF	16							13
DCF	459	32	1310	180	4-6		primary sludge	14
DCF	16	3	47	32	4-6		secondary sludge	14

Compound	K <sub>D</sub> (L/kg)		K <sub>oc</sub> (L/kg)		Replicates	f <sub>oc</sub> (%)	Sludge name / comments	Reference
	value	(s.d.)	value	(s.d.)				
E2	476	192	1738		9		K <sub>f</sub> units l <sup>n</sup> ng <sup>(1-n)</sup> kg <sup>-1</sup>	16
E2	461	212	2004			18 - 28	no pre-treatment	9
E2	200		685			29.2	ozone	9
E2	229				4		Primary (mean)	17
E2	151				4		WAS (mean)	17
E2	17				1		drum thickener (BNR)	17
E2	692		1995				K <sub>f</sub> units mg <sup>(1-1/n)</sup> L <sup>(1/n)</sup> g <sup>-1</sup>	18
E2	183	12						19
E2	604						15 °C	20
E2	487						25 °C	20
E2	312						35 °C	20
E2	245						45 °C	20
E2	458	20	1549	32	6	29.7		21
E2	154	309						22
E2	230						Secondary sludge, long sludge	23
E2	771	108	1698					4
E2	560	67	1122					4
E2	522	34	1175					4
E2	631							13
E2	403	69			3		activated sludge 20 °C	24
E2	485	50					activated sludge 10 °C	23
E2	350	76					activated sludge 30 °C	23
E2	698	17					10 days anaerobic unit	25
E2	529	13					10 days anoxic unit	24
EE2	584	136	2089		9		K <sub>f</sub> units l <sup>n</sup> ng <sup>(1-n)</sup> kg <sup>-1</sup>	16
EE2	432	168	1878			18 - 28	no pre-treatment	9
EE2	387	84	2224			11 - 23.8	alkaline	9
EE2	200		685			29.2	ozone	9
EE2	4571				4		primary (mean)	17
EE2	575				4		WAS (mean)	17
EE2	776				1		drum thickener (BNR)	17
EE2	692		2042				K <sub>f</sub> units mg <sup>(1-1/n)</sup> L <sup>(1/n)</sup> g <sup>-1</sup>	18
EE2	281	22						19
EE2	631						15 °C	20
EE2	508						25 °C	20
EE2	337						35 °C	20
EE2	267						45 °C	20
EE2	582	1	1827	1	6	29.7		21
EE2	575	1085						22

Compound	K <sub>D</sub> (L/kg)		K <sub>OC</sub> (L/kg)		Replicates	foc (%)	Sludge name / comments	Reference
	value	(s.d.)	value	(s.d.)				
EE2	1550	223	3467					4
EE2	1017	105	2042					4
EE2	1103	76	2455					4
EE2	316							13
EE2	278	3	794	95	4-6		primary sludge	14
EE2	349	37	860	140	4-6		secondary sludge	14
EE2	3236						MBR 22 °C in time series	26
EE2	2818						MBR 24 °C in time series	25
EE2	1622						SBR 22 °C in time series	25
EE2	1479						SBR 24 °C in time series	25
EE2	2951						adsorption MBR	27
EE2	3631						desorption MBR	26
EE2	2089						adsorption CBR	26
EE2	4074						desorption CBR	26
EE2	741	9					10 days anaerobic unit	24
EE2	623	6					10 days anoxic Unit	24
EE2	613	4					10 days oxic Unit	24
EE2	2595						primary sludge adsorption	28
EE2	2824						primary sludge desorption	27
EE2	1979						anaerobic sludge absorption	27
EE2	2499						anaerobic sludge desorption	27
SMX	23		100			18 - 28	no pre-treatment	9
SMX	62		353			11 - 23.8	alkaline	9
SMX	10		42			19.6 -26.2	thermal	9
SMX	256	169			9-15			29
SMX	114				1			28
SMX	400				1			28
SMX	269	43	617		6	44.1		10
SMX	400	2					primary sludge	30
SMX	260	2					standard WTP sludge	29
SMX	260	2					membrane bioreactor sludge	29
SMX	63						min thickened sludge	6
SMX	398						max thickened sludge	6
SMX	3	5			7		primary sludge	12
SMX	77	70			7		second activation	12
SMX	60	49			7		FS MBR	12
SMX	63	42			7		HF MBR	12
SMX	320						primary sludge	23
SMX	370						secondary sludge, short sludge	23

Compound	K <sub>d</sub> (L/kg)		K <sub>oc</sub> (L/kg)		Replicates	f <sub>oc</sub> (%)	Sludge name / comments	Reference
	value	(s.d.)	value	(s.d.)				
SMX	370						secondary sludge, long sludge	23
SMX	29	2	38	3			adsorption	31
SMX	47						desorption (NaN <sub>2</sub> dosed)	30
SMX	32	1	62	1			sorption	32
SMX	44						desorption	31
SMX	<30						Denver Metro AS	4
SMX	<30						Denver Metro Primary	4
SMX	<30						Mines Park AS	4



**Figure S19.** Comparison of average literature log  $K_{oc}$  values and standard deviations (error bars) and those measured in this study for the test analytes. For caffeine and norethindrone, no log  $K_{oc}$  values in the literature could be found. The largest significant discrepancy is for sulfamethoxazole, which is due to  $K_{oc}$  data being available largely from the most sorbing of sludges. The consistently smaller  $K_{oc}$  for a alum sludges is a preliminary indication that the OC content may not be the only reason alum sludges sorb less.

## S9. References

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