Supplementary Information

Modeling Risk Dynamics of Contaminants of Emerging Concern in a Temperate-region Wastewater Effluent-dominated Stream

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CONTAINS:

Field site details, chemical details, 18 Supporting Tables, 11 Supporting Figures, Supporting References, 23 pages in total.

SUPPORTING METHODS

Table S.1: Land use information from Muddy Creek.[1]

Station Name	Open Water	Developed	Barren Land (Rock/Sand/ Clay)	Forest	Shrub/ Scrub	Grassland/ Herbaceous	Pasture/ Hay	Cultivated Crops	Wetlands
US1 (05454050)	0.13%	72.5%	0.07%	1.69%	0%	1.61%	2.82%	20.72%	0.44%
Effluent (05454051)	0.13%	72.5%	0.07%	1.70%	0%	1.61%	2.81%	20.69%	0.46%
DS1 (05454052)	0.13%	72.3%	0.07%	2.0%	0%	1.60%	2.86%	20.52%	0.47%
DS2 (05454090)	0.40%	60.0%	0.04%	12.4%	0.02%	2.38%	7.06%	17.45%	0.31%

Data from USGS National Landcover Database (2019).

Table S.2: Sampling timelines of monitoring contaminants of emerging concern (CECs). One data set consisted of four samples from each of the four sampling sites (US1, Effluent, DS1 and DS2)

Chemical	Frequency	Data sets	Year 1 (September 2017- August 2018)	Year 2 (September 2018- August 2019)
Pharmaceuticals and atrazine[2]	monthly	12		
Pharmaceuticals and industrial chemicals[1]	monthly	12		
Pharmaceuticals and industrial chemicals	Three times per day	12		July 14-July 18, 2019
Neonicotinoids[3]	biweekly	17		
Pharmaceuticals and industrial chemicals in drinking water	one time	2 (1 for influent, 1 for effluent)		May 12, 2018

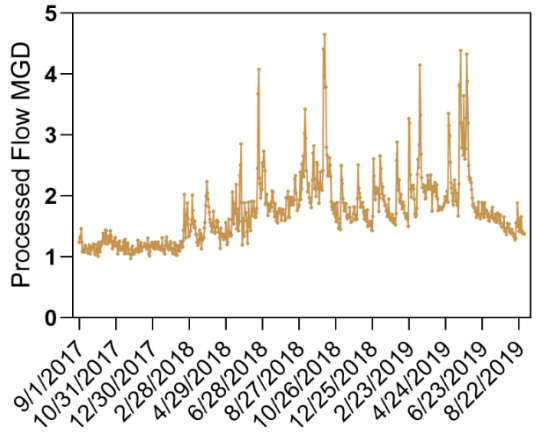

Figure S.1: Wastewater treatment plant (WWTP) daily processed flow discharges during September 2017- August 2019. Data were provided by the North Liberty WWTP.[1]

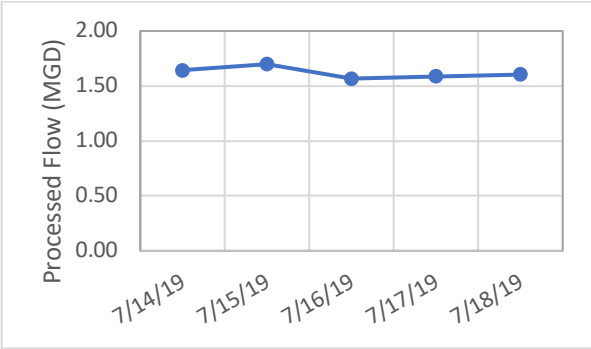

Figure S.2: Daily processed flow in North Liberty Wastewater treatment during July 14–July 18, 2019.

Table S.3: Chemical properties of CECs investigated in the present study.

	Category	CAS	logKow§	pKa§	LogKoc[4]	Predicted biodegradation half-lives (d)[5]	Photolysis half-lives (d)
Venlafaxine	Antidepressant pharmaceutical	93413-69-5	3.28	14.4; 8.9	3.2	3.36	2.4–15[6,7]
Desvenlafaxine	Antidepressant pharmaceutical	93413-62-8	0.74	8.9; 10.1	3.5	4.66	0.75[7]
Metformin	Antidiabetic pharmaceutical	657-24-9	-2.64	12.3	2.1	3.98	negligible[8]
Guanylurea	Metformin metabolite	141-83-3	-2.51	8.0; 13.5	2.0	4.10	negligible[9]
Fluconazole	Anti-fungal pharmaceutical	86386-73-4	0.25	12.7	NA	4.46	0.08[10]
Bupropion	Antidepressant pharmaceutical	34911-55-2	3.85	7.2	3.0	3.39	negligible[11]
Citalopram	Antidepressant pharmaceutical	59729-33-8	3.74	9.5	4.4; 5.6[12]	3.55	negligible[6]
Atenolol	Beta-blocker pharmaceutical	29122-68-7	0.16	9.6	2.17	3.34	3.2–30.4[13]
Carbamazepine	Anti-seizure pharmaceutical	298-46-4	2.45	15.9	3.6	5.03	3.5–416[13–15]
Tramadol	Pain-relief pharmaceutical	27203-92-5	3.01	9.2; 13.8	2.79	3.35	3.04[7]
Sulfamethoxazole	Antibiotic pharmaceutical	723-46-6	0.89	1.9; 6.2; 0.3	1.86	3.34	2.4–6.1[14,15]
Fexofenadine	Antihistamine pharmaceutical	83799-24-0	0.3	8.8; 4.3	1.54	26.2	4.4–6.8[14]
Methocarbamol	Muscle relaxer pharmaceutical	532-03-6	0.61	13.6	1.7	4.48	NA
Lidocaine	Anesthetic pharmaceutical	137-58-6	2.26	7.7; 13.8	2.6	3.36	1.3[7]
1H-benzotriazole	industrial chemical	95-14-7	1.44	8.4	1–2.7	3.99	9.0 ± 0.3[16]
5-methyl-benzotriazole	industrial chemical	136-85-6		8.8	2.04	2.53	2.5 ± 0.1[16]
Atrazine	Herbicide	1912-24-9	2.68	1.68	1.96–3.38	4.91	
Clothianidin	Neonicotinoid pesticide	210880-92-5	0.7	11.09	1.78	3.55	
Imidacloprid	Neonicotinoid pesticide	138261-41-3	0.57	11.12	2.56	3.54	
Thiamethoxam	Neonicotinoid pesticide	153719-23-4	-0.13	0.41	1.84	4.45	

(§ citation for pKa, logKow: Kim et al.[17]; NA: not available)

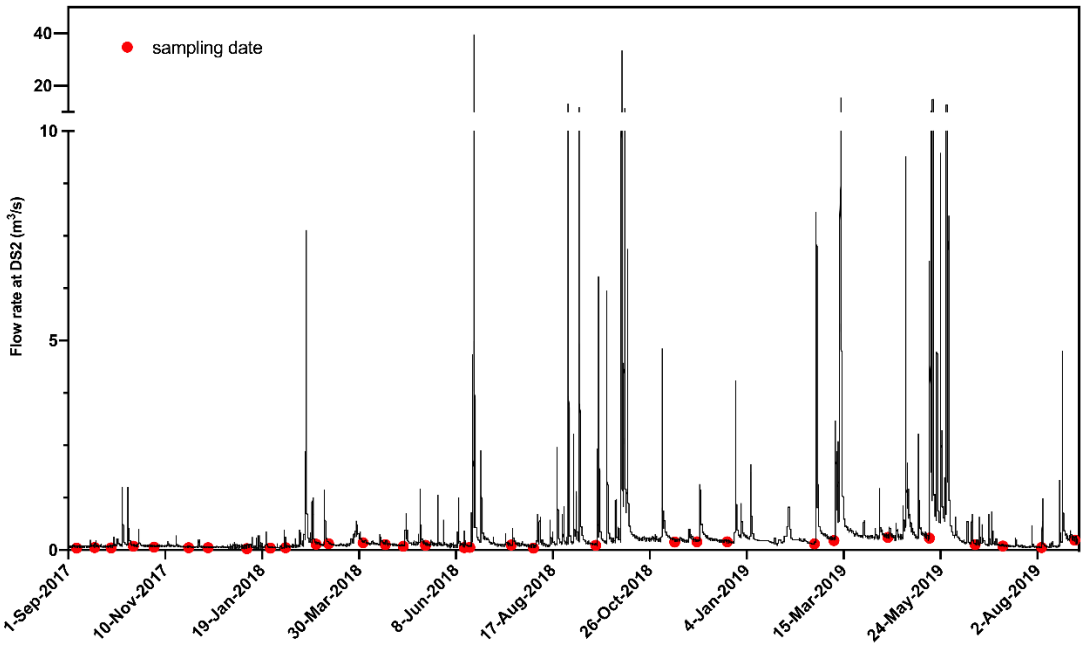

Figure S.3: Two-year diurnal hydrograph at DS2 (Station ID 05454090).[1,2] Red dots represent dates when sampling events occurred (n=37). All samples were collected during baseflow conditions.

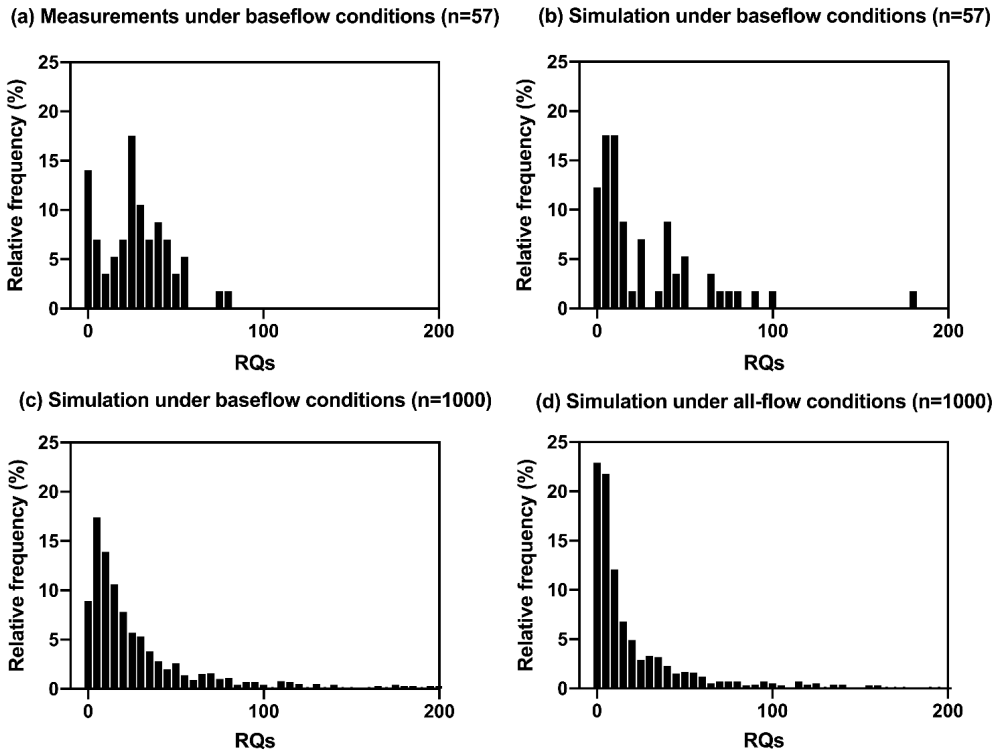

Figure S.4: Example of Monte Carlo simulation of risk quotients (RQs). (a) RQs relative frequency from our field measured data fexofenadine under baseflow conditions (n=57); (b) Simulated RQs relative frequency under baseflow conditions (n=57); (c) Simulated RQs relative frequency under baseflow conditions (n=1000); (d) Simulated RQs relative frequency percentage under all-flow conditions (n=1000).

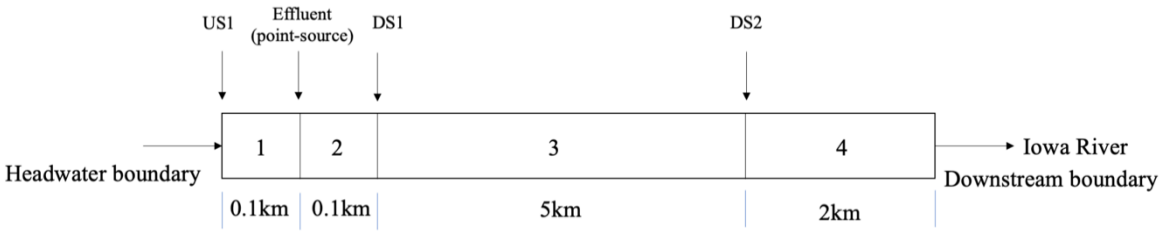

Figure S.5: System segmentation of Muddy Creek field site in QUAL2K modeling.

A steady-state flow balance is implemented for each model element. Once the flow of an element has been solved, the velocity and depth are calculated using the empirically derived rating curves as proposed by Leopold and Maddock[18]:

$$U = aQ^b \qquad \text{S.1}$$

$$H = \alpha Q^\beta \qquad \text{S.2}$$

where U is flow velocity (m/s), Q is flow rate (m3/s), H is water depth (m) and a, b, α and β are empirical coefficients that can be determined from the hydraulic measurements and stream geometry.

SUPPORTING RESULTS

Table S.4: Median lethal dose (LC50) values or half-maximal effective concentration values (EC50; in mg/L) that were used to calculate predicted no-effect concentration (PNEC; in µg/L) (by dividing LC50 or EC50 by an assessment factor of 1000) for fish, invertebrate (mostly Daphnia magna), and algae for acute effects. Toxicity data were selected based on Table S.5.

Compound	EC50/LC50 (mg/L)			PNEC (µg/L)		
	Algae	Invertebrate	Fish	Algae	Invertebrate	Fish
Atenolol	2337	6799	14438	2337	6799	14438
Atrazine	0.042	0.24	6.21	0.042	0.24	6.21
Bupropion	0.36	0.48	3.23	0.36	0.48	3.23
Carbamazepine	27	27	22	27	27	22
Citalopram	0.36	0.65	4.5	0.36	0.65	4.5
Clothianidin	56	0.0024	101.5	56	0.0024	101.5
Desvenlafaxine	32.3	33	9.4	32.3	33	9.4
Fexofenadine	200	780	940	200	780	940
Fluconazole	–	–	–	–	–	–
Guanylurea	–	–	–	–	–	–
Imidacloprid	10	0.0015	9.02	0.0055	0.0015	277
Lidocaine	0.64	6.2	56.2	0.64	6.2	56.2
Metformin	110	32	982	110	64	14034
Methocarbamol	962	1770	643	962	1770	643
Sulfamethoxazole	0.027	4.5	56.2	0.027	4.5	56.2
Thiamethoxam	81.8	0.024	80	81.8	0.024	80
Tramadol	0.82	1.41	11.4	0.82	1.41	11.4
Venlafaxine	13	10	16	13	10	16
1H-benzotriazole	5.9	66.8	28	5.9	66.8	28
5-methyl-benzotriazole	23.2	50.89	22	23.2	50.89	22

Note: "-" indicates data unavailable.

Table S.5: Median lethal dose (LC50) or half-maximal effective concentration (EC50) (in mg/L) based on acute effects are used to calculate predicted no-effect concentration (PNEC) (by dividing LC50 or EC50 by an assessment factor of 1000) for fish, invertebrate, and algae.

Compound	EC50/LC50 (mg/L)		
	Algae	Invertebrate	Fish
Atenolol	2337[19]	6799[19]	14438[19]
Atrazine	0.042–0.104[20,21]	0.24-29[21–23]	6.21–12.9[24]
Bupropion	0.36[25]	0.48[25]	3.23-503[25,26]
Carbamazepine	27[27]	27[27]	22[27]
Citalopram	0.36[19]	0.65[19]	4.5[19]
Clothianidin	56[28]	2.41 µg/L-119[28,29]	101.5[28]
Desvenlafaxine	32.3[21]	33[21]	9.4[21]
Fexofenadine	200[30]	780[30]	940[30]
Fluconazole	–	–	–
Guanylurea	–	–	–
Imidacloprid	10[21]	1.52 µg/L-85 [21,29,31–33]	9.02-277[21,32,34]
Lidocaine	0.64-140[19,25]	6.2-215[19,25]	56.2-390[19,25]
Metformin	110-320[21,35]	32-64[21,36]	982-14034[21,25]
Methocarbamol	962[25]	1770[25]	643[25]
Sulfamethoxazole	0.027[37]	4.5[38]	56.2[39]
Thiamethoxam	81.8[21,40]	0.014-100[21,29,40]	80-100[32,40]
Tramadol	0.82-8.7[25,27]	1.41-28[25,27]	11.4-70[25,27]
Venlafaxine	13-66[19,25]	10-140[19,21,25]	16-249[19,25]
1H-benzotriazole	5.9–156.16[21,41–43]	66.8–288.14[21,41–45]	28–548.05[21,41,42,46,47]
5-methyl-benzotriazole	23.2–72.96[42,43,48]	50.89–109.24[42,43,45,48]	22–197.53[42,46–50]

Table S.6: Chronic toxicity data used for risk assessment selected based on Table S.7. An assessment factor of 10 was applied to calculate PNEC values.

Compound	NOEC/LOEC/EC10 (mg/L)			PNEC(µg/L)		
	Algae	Invertebrate	Fish	Algae	Invertebrate	Fish
1H-benzotriazole	1.18	0.97	46	118	97	4600
5-methyl-benzotriazole	2.11	0.4	11	211	40	1100
Clothianidin	–	0.28 µg/L	9.7	–	0.028	970
Imidacloprid	30 ng/L	1.8–42	50	0.003	180	5000
Thiamethoxam	81.8	0.3 µg/L	20	8180	0.03	2000
Atrazine	0.011	29	100 µg/L	1.1	2900	10

Note: "-" indicates data not available.

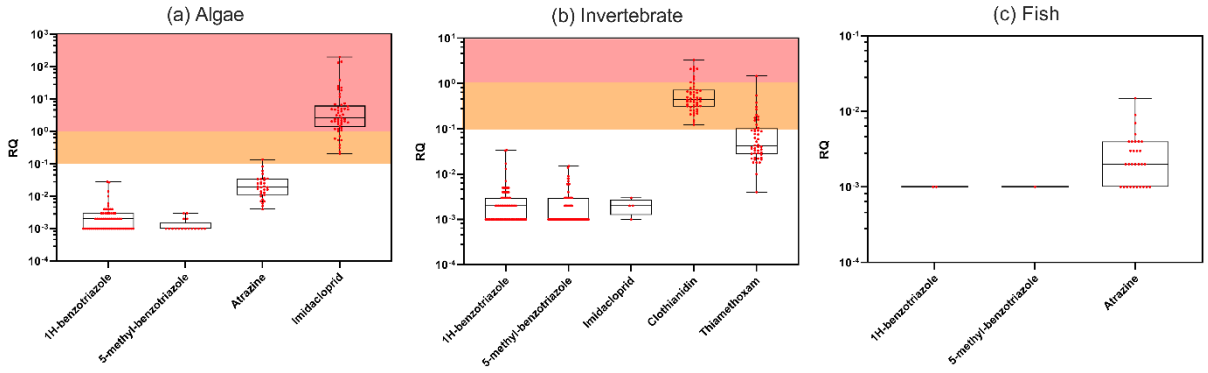

Figure S.6: Measured risk quotients (RQs) for algae (a), invertebrates (b) and fish (c) of industrial chemicals and pesticides aggregated from all three in-stream sites (US1, DS1, DS2) based on **chronic toxicity data** in Muddy Creek. RQs $<10^{-4}$ were considered negligible risks and were not included in the figure. Chemicals not present in the figure were due to all RQs were $<10^{-4}$. The chronic toxicity data of clothianidin to algae were not available based on our literature search. Red shade indicates high risk (RQ≥1), orange shade indicates medium risk (0.1≤RQ<1), no shade indicates low risks. The box and whiskers from bottom to top represent minimum value, 25th percentile, median value, 75th percentile and maximum value.

Table S.7: Toxicity data for industrial chemicals and pesticides.

Compound	Class	Species	Duration	Effect	Guideline	Endpoint	Value (mg/L)	Reference
1H-benzotriazole	Algae	*Desmodesmus subspicatus*	72h	-	OECD 201	NOEC/ EC10	1.18	[21]
1H-benzotriazole	Algae	*Lemna minor*	7d	-	OECD 201	EC10	3.94	[21]
1H-benzotriazole	Invertebrate	*Daphnia galeata*	21d	-	OECD 201	EC10	0.97	[21]
1H-benzotriazole	Fish	*Danio rerio*	96h	Mortality	USEPA	NOAEC	46	[47]
1H-benzotriazole	Fish	*Danio rerio*	96h	Mortality	USEPA	LOAEC	92	[47]
5-methyl-benzotriazole	Algae	*Desmodesmus subspicatus*	72h	-	OECD 201	EC10	2.86	[21]
5-methyl-benzotriazole	Algae	*Lemna minor*	7d	-	OECD 201	EC10	2.11	[21]
5-methyl-benzotriazole	Invertebrate	*Daphnia magna*	21d	Reproduction	OECD 201	NOAEC	6.4	[43]
5-methyl-benzotriazole	Invertebrate	*Daphnia galeata*	21d	Reproduction	OECD 201	NOAEC	1	[43]
5-methyl-benzotriazole	Invertebrate	*Daphnia galeata*	21d	Reproduction	OECD 201	LOAEC	2	[43]
5-methyl-benzotriazole	Invertebrate	*Daphnia galeata*	21d	-	OECD 201	EC10	0.4	[21]
5-methyl-benzotriazole	Invertebrate	*Ceriodaphnia dubia*	48h	Mortality	USEPA	NOAEC	47	[47]
5-methyl-benzotriazole	Invertebrate	*Ceriodaphnia dubia*	48h	Mortality	USEPA	LOAEC	94	[47]
5-methyl-benzotriazole	Invertebrate	*Ceriodaphnia dubia*	48h	Mortality	USEPA	NOAEC	47	[47]
5-methyl-benzotriazole	Fish	*Pimephales promelas (Fathead minnows)*	96h	Mortality	USEPA	NOAEC	11	[47]
5-methyl-benzotriazole	Fish	*Pimephales promelas (Fathead minnows)*	96h	Mortality	USEPA	LOAEC	24	[47]
Imidacloprid	Algae	*Tetraedon sp.*	72h	Biomass	OECD 201	NOEC	30 ng/L	[51]
Imidacloprid	Algae	-	72h	Growth rate	OECD 201	NOEC	10	[21]
Imidacloprid	Invertebrate	-	21d	-	OECD 201	NOEC	1.8	[21]
Imidacloprid	Invertebrate	-	48h	-	OECD 201	NOEC	42	[21]
Imidacloprid	Invertebrate	*Chironomus dilutus*	96h	-	USEPA	EC10	0.13 µg/L	[52]
Imidacloprid	Invertebrate	*Neocloeon triangulifer*	96h	-	USEPA	EC10	1.12 µg/L	[52]
Imidacloprid	Fish	*Oncorhynchus mykiss (Rainbow Trout)*	96h		OECD 201	NOEC	50	[21]

Clothianidin	Algae	-	-	-	-	-	-	-
Clothianidin	Invertebrate	*Chironomus dilutus*		-	USEPA	EC10	0.42 µg/L	[52]
Clothianidin	Invertebrate	*Neocloeon triangulifer*		-	USEPA	EC10	0.28 µg/L	[52]
Clothianidin	Fish	*Pimephales promelas (Fathead minnows)*		-	USEPA	NOEC	9.7	[53]
Thiamethoxam	Invertebrate	*Cloeon dipterum*		-	OECD 2006	NOEC	0.3 µg/L	[21]
Thiamethoxam	Invertebrate	*Chironomus dilutus*		-	USEPA	EC10	11.15 µg/L	[52]
Thiamethoxam	Fish	*Oncorhynchus mykiss (Rainbow Trout)*	88d	-	OECD 201	NOEC	20	[21]
Atrazine	Algae	*Desmodesmus subspicatus*	72h	-	OECD 201	NOEC	0.011	[21]
Atrazine	Invertebrate	*Daphnia magna*	40h	Visual inspection	OECD 201	NOEC	29	[21]
Atrazine	Fish	-		-	USEPA	LOEC	100 µg/L	[54]

Table S.8 (a-c): RQs of acute effect from measured field data under baseflow conditions for algae, invertebrate and fish. "-" indicated RQs $<10^{-4}$.

(a) Algae

RQs	Max	Median	Min	Mean	Std.
1H-benzotriazole	0.556	0.027	0.002	0.052	0.094
5-methyl-benzotriazole	0.026	0.002	0.001	0.004	0.005
Atrazine	3.571	0.495	0.115	0.695	0.687
Bupropion	1.466	0.466	0.101	0.534	0.307
Carbamazepine	0.017	0.008	0.002	0.008	0.004
Citalopram	1.541	0.101	0.005	0.355	0.392
Clothianidin	0.002	0.001	0.001	0.001	0.000
Desvenlafaxine	0.055	0.011	0.001	0.020	0.016
Fexofenadine	0.020	0.007	0.001	0.008	0.004
Imidacloprid	0.060	0.001	0.001	0.006	0.013
Lidocaine	0.742	0.163	0.008	0.240	0.204
Metformin	0.108	0.006	0.001	0.009	0.014
Methocarbamol	0.398	0.058	0.006	0.083	0.075
Sulfamethoxazole	51.111	7.678	0.018	12.319	12.656
Thiamethoxam	0.001	0.001	0.001	0.001	0.000
Tramadol	0.624	0.133	0.003	0.215	0.190
Venlafaxine	0.087	0.040	0.008	0.042	0.021

(b) Invertebrate

RQ	Max	Median	Min	Mean	Std.
1H-benzotriazole	0.049	0.003	0.001	0.005	0.009
5-methyl-benzotriazole	0.012	0.001	0.001	0.002	0.002
Atrazine	0.625	0.087	0.020	0.122	0.120
Bupropion	1.100	0.349	0.075	0.400	0.230
Carbamazepine	0.017	0.008	0.002	0.008	0.004
Citalopram	0.853	0.056	0.003	0.196	0.217
Clothianidin	38.667	5.125	1.442	8.118	7.718
Desvenlafaxine	0.054	0.011	0.001	0.019	0.016
Fexofenadine	0.005	0.002	0.001	0.002	0.001
Imidacloprid	400.667	5.207	0.413	28.040	73.520
Lidocaine	0.077	0.017	0.001	0.025	0.021
Metformin	0.372	0.020	0.001	0.029	0.049
Methocarbamol	0.216	0.030	0.001	0.044	0.041
Sulfamethoxazole	0.307	0.046	0.001	0.074	0.076
Thiamethoxam	1.825	0.052	0.005	0.145	0.277
Tramadol	0.363	0.077	0.002	0.125	0.110
Venlafaxine	0.113	0.052	0.010	0.054	0.027

(c) Fish

RQ	Max	Median	Min	Mean	Std.
1H-benzotriazole	0.117	0.006	0.001	0.011	0.020
5-methyl-benzotriazole	0.028	0.002	0.001	0.004	0.005
Atrazine	0.024	0.003	0.001	0.005	0.005
Bupropion	0.163	0.052	0.011	0.059	0.034
Carbamazepine	0.021	0.009	0.002	0.010	0.005
Citalopram	0.123	0.009	0.001	0.029	0.031
Clothianidin	0.001	0.001	0.001	0.001	0.000
Desvenlafaxine	0.190	0.038	0.001	0.064	0.057
Fexofenadine	0.004	0.002	0.001	0.002	0.001
Imidacloprid	0.067	0.002	0.001	0.006	0.014
Lidocaine	0.008	0.003	0.001	0.003	0.002
Metformin	0.012	0.001	0.001	0.002	0.002
Methocarbamol	0.596	0.086	0.010	0.124	0.112
Sulfamethoxazole	0.025	0.004	0.001	0.006	0.006
Thiamethoxam	0.001	0.001	0.001	0.001	0.000
Tramadol	0.045	0.010	0.001	0.016	0.014
Venlafaxine	0.071	0.032	0.007	0.034	0.017

Table S.9: Inputs of RQs inputs for Monte Carlo simulation. "-" indicated RQ<0.1. Data are based on acute effect and are post log-transformed.

RQ	Algae		Invertebrate		Fish	
	Mean	Std.	Mean	Std.	Mean	Std.
Bupropion	-0.79	0.59	-1.08	0.60	-	-
Citalopram	-1.79	1.35	-2.38	1.35	-	-
Clothianidin	-	-	1.78	0.75	-	-
Desvenlafaxine	-	-	-	-	-3.37	1.38
Imidacloprid	-	-	1.91	1.49	-	-
Lidocaine	-1.97	1.18	-	-	-	-
Methocarbamol	-	-	-	-	-2.43	0.83
Sulfamethoxazole	1.87	1.37	-3.21	1.23	-	-
Thiamethoxam	-	-	-2.65	1.08	-	-
Tramadol	-2.11	1.26	-2.65	1.25	-	-

Table S.10: Inputs of stream flow rate inputs at DS2 for Monte Carlo simulation (unit: m^3/s). Data were post log-transformed.

	Mean	Std.
Baseflow condition	-2.20	0.61
All-flow condition	-1.64	0.89

Table S.11: Risk quotients of acute effect from simulations for both baseflow conditions and all-flow conditions.

RQs	Baseflow conditions					All-flow conditions				
	Mean	std.	median	75th percentile	90th percentile	Mean	std.	median	75th percentile	90th percentile
Algae										
Bupropion	0.53	0.34	0.44	0.67	0.93	0.54	0.88	0.27	0.59	1.24
Citalopram	0.44	0.88	0.18	0.45	1.06	0.50	1.98	0.10	0.36	0.98
Lidocaine	0.29	0.41	0.15	0.34	0.71	0.31	0.78	0.09	0.27	0.68
Sulfamethoxazole	17.21	63.55	6.17	15.36	37.29	18.18	71.11	3.73	12.36	31.98
Tramadol	0.25	0.48	0.12	0.27	0.53	0.25	0.75	0.06	0.20	0.55
Invertebrate										
Bupropion	0.40	0.26	0.34	0.50	0.72	0.41	0.72	0.19	0.43	0.92
Citalopram	0.23	0.38	0.10	0.25	0.55	0.26	0.87	0.05	0.19	0.53
Clothianidin	7.90	6.69	5.81	10.37	15.83	8.09	16.31	3.62	7.61	18.72
Imidacloprid	21.98	59.24	6.79	18.93	46.80	28.31	179.94	3.88	15.12	46.54
Sulfamethoxazole	0.08	0.12	0.04	0.10	0.20	0.08	0.17	0.02	0.07	0.22
Thiamethoxam	0.12	0.15	0.07	0.15	0.28	0.12	0.25	0.04	0.11	0.31
Tramadol	0.17	0.33	0.07	0.16	0.37	0.21	0.86	0.04	0.13	0.36
Fish										
Desvenlafaxine	0.08	0.17	0.04	0.08	0.18	0.09	0.29	0.02	0.07	0.17
Methocarbamol	0.13	0.14	0.09	0.16	0.27	0.13	0.32	0.05	0.13	0.28

Table S.12 (a-c): RQs of chronic effect from measured field data under baseflow conditions for algae, invertebrate and fish. "-" indicated RQs $<10^{-4}$.

(a) Algae

RQs	Max	Median	Min	Mean	Std.
1H-benzotriazole	0.028	0.002	0.001	0.003	0.005
5-methyl-benzotriazole	0.003	0.001	0.001	0.001	0.001
Clothianidin	-	-	-	-	-
imidacloprid	200.333	2.603	0.207	14.020	36.760
Thiamethoxam	-	-	-	-	-

(b) Invertebrate

RQs	Max	Median	Min	Mean	Std.
1H-benzotriazole	0.034	0.002	0.001	0.003	0.006
5-methyl-benzotriazole	0.015	0.001	0.001	0.002	0.003
Clothianidin	3.314	0.439	0.124	0.696	0.662
Imidacloprid	0.003	0.002	0.001	0.002	0.001
Thiamethoxam	1.460	0.042	0.004	0.116	0.222

(c) Fish

RQs	Max	Median	Min	Mean	Std.
1H-benzotriazole	0.001	0.001	0.001	0.001	-
5-methyl-benzotriazole	0.001	0.001	0.001	0.001	-
Clothianidin	-	-	-	-	-
Imidacloprid	-	-	-	-	-
Thiamethoxam	-	-	-	-	-

Table S.13: Inputs of RQs inputs for Monte Carlo simulation. "-" indicated RQ<0.1. Data are based on chronic effect and are post log-transformed.

RQ	Algae		Invertebrate		Fish	
	Mean	Std.	Mean	Std.	Mean	Std.
1H-benzotriazole	-	-	-	-	-	-
5-methyl-benzotriazole	-	-	-	-	-	-
Clothianidin	-	-	-0.68	0.75	-	-
Imidacloprid	1.22	1.49	-	-	-	-
Thiamethoxam	-	-	-2.88	1.09	-	-

Table S.14: Risk quotients of chronic effect from simulations for both baseflow conditions and all-flow conditions.

RQs	Baseflow conditions					All-flow conditions				
	Mean	std.	median	75th percentile	90th percentile	Mean	std.	median	75th percentile	90th percentile
Algae										
Imidacloprid	10.56	32.44	3.49	9.24	24.00	10.46	38.05	2.05	6.78	20.07
Invertebrate										
Clothianidin	0.71	0.60	0.54	0.89	1.45	0.66	1.28	0.30	0.70	1.54
Thiamethoxam	0.10	0.14	0.05	0.11	0.22	0.10	0.21	0.03	0.09	0.23

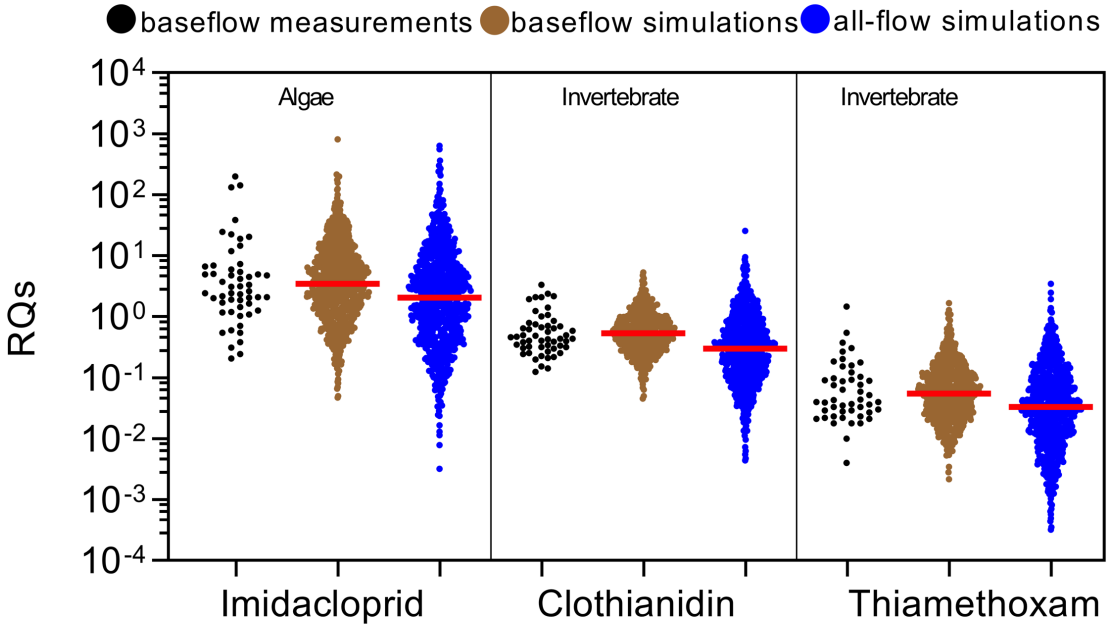

Figure S.7: Measured and simulated risk quotients (RQs) of chronic effect for stochastic risk modeling. Measured values occurred under baseflow conditions, whereas the simulated conditions were generated via Monte Carlo simulations for baseflow and all flows during the two-year sampling period (flows determined at site DS2 using the USGS flow gage). Red solid lines represent median values for each data set. Compounds were selected for stochastic risk simulation when the 75th percentile of the total measured RQs under baseflow conditions exceeded the lowest problematic risk level (i.e., RQ=0.1) for at least one of the three different aquatic species types (i.e., algae, invertebrates, fish). Only imidacloprid exhibited medium or higher risks to algae, and only two compound clothianidin and thiamethoxam exhibited medium or higher risks to invertebrate.

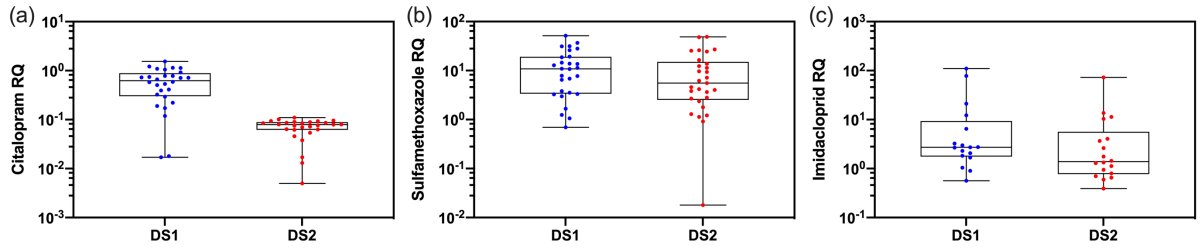

Figure S.8: Risk quotients (RQs) comparison of pharmaceutical (a) citalopram, (b) sulfamethoxazole and (c) imidacloprid from baseflow measurements at sites DS1 and DS2 in Muddy Creek (Coralville, Iowa). For citalopram, a rapidly-attenuated compound in the stream, the RQs at DS1 were significantly higher than RQs at DS2 ($p<0.0001$), whereas for other two compounds, the RQs at DS1 were not significantly different from RQs at DS2 ($p>0.05$). The box and whiskers from bottom to top represent minimum value, 25th percentile, median value, 75th percentile and maximum value.

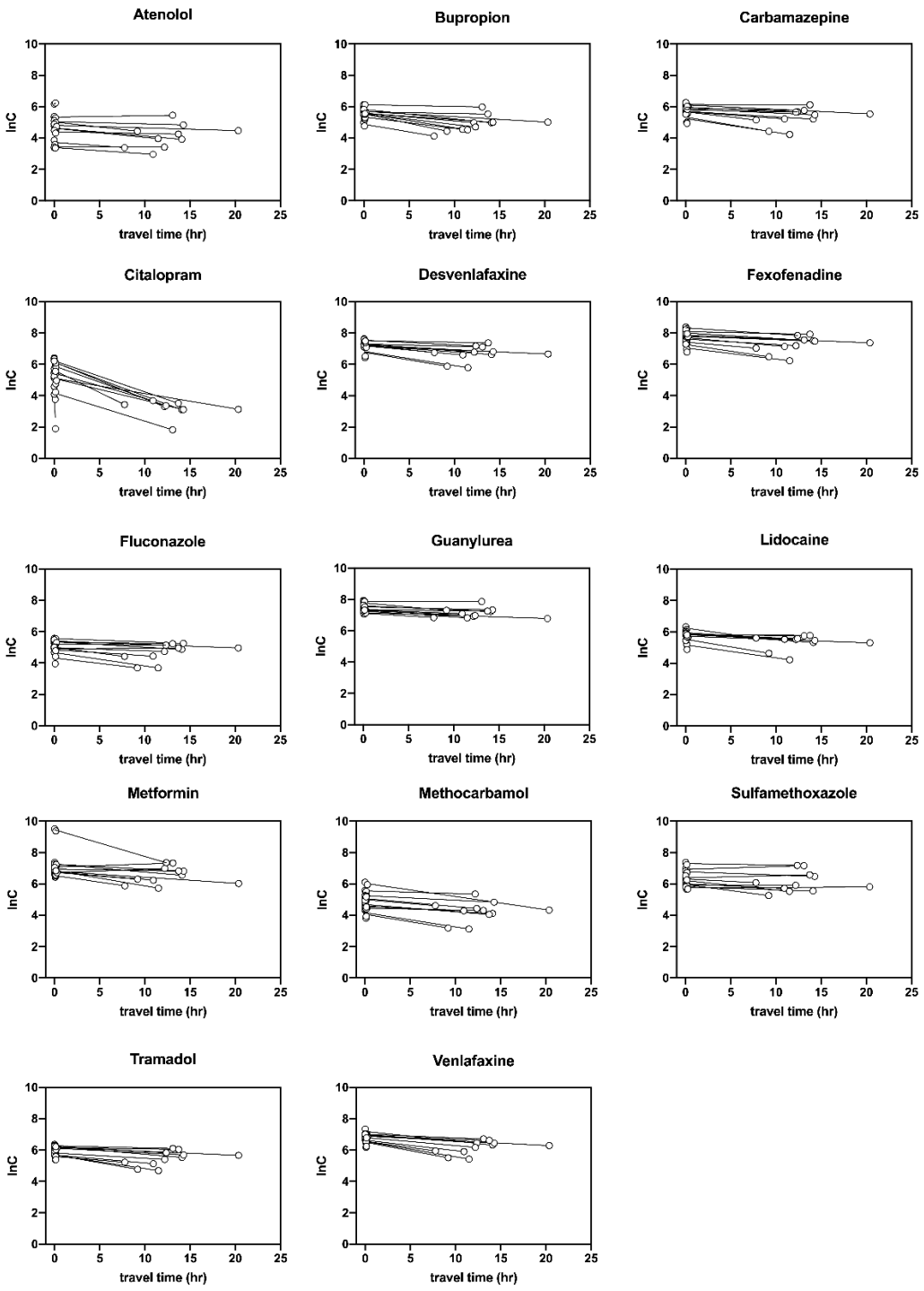

Figure S.9: The first order in-stream attenuation of pharmaceutical compounds. Black open circles represent individual field measurement. Each slope represents the rate constant for each sampling set during September 2017–August 2018.[2] All the rate constants can be found in Table S.6. The x-axis is the travel time calculated based on travel distance and measured flow velocity.[2] Stream stage at DS2 was continuously monitored by the USGS gaging station (05454090) to calculate flow based on a stage/discharge rating curve developed for this specific site.[55] The estimated width of the streambed at DS2 is 4 m.

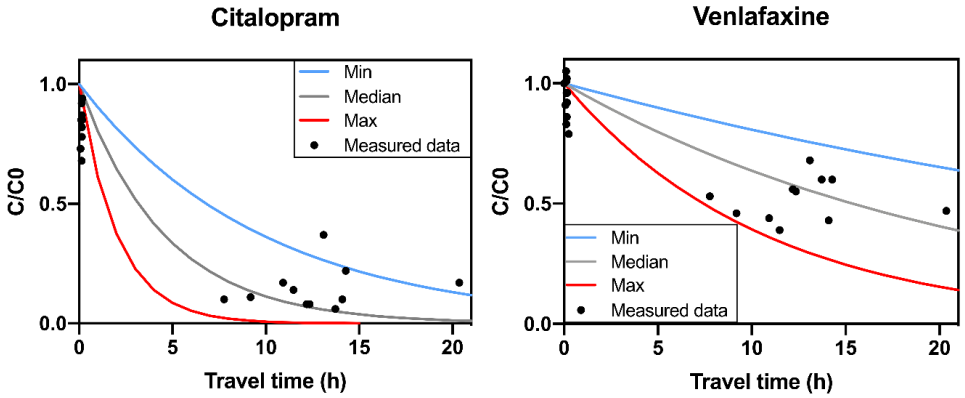

Figure S.10: Model calibration and validation for pharmaceuticals citalopram and venlafaxine. U.S. Geological Survey monthly data collected from Muddy Creek (Coralville, Iowa) during Year 1 were used for model calibration. Simulation results are based on the maximum, median and minimum rate constants. University of Iowa monthly data during Year 1 (September 2017 – August 2018) were used for model validation, shown as 'measured data' here in the figure.

Table S.15: Stream flow data provided by U.S. Geological Survey during September 2017 to August 2018.[2] * indicates water was frozen, so the measurement is questionable. # indicates estimated value by U.S. Geological Survey; the streamflow measurement for US1 for January was inadvertently deleted prior to formal documentation and was estimated by using available streamflow measurements from the December 2017 (US1 and DS1) to January 2018 (DS1) and by comparing photos from December 2017 and January 2018 at US1. The median estimated travel time to Iowa River is 37.91h.

Date	DS1			DS2				Estimated travel time to Iowa River (h)
	Flow rate (m^3/s)	Velocity (m/s)	Estimated travel time (h)	Flow rate (m^3/s)	Height (m)	Estimated velocity (m/s)	Estimated travel time (h)	
2017/9/7	0.083	0.21	0.13	0.048	0.67	0.018	12.35	43
2017/10/2	0.065	0.18	0.15	0.054	0.68	0.020	13.72	41
2017/11/2	0.050	0.11	0.25	0.072	0.71	0.025	20.36	42
2017/12/11	0.094	0.18	0.16	0.051	0.70	0.018	14.28	45
2018/1/8	0.10#	0.22	0.12	0.033*	0.68	NA	NA	NA
2018/2/5	0.086	0.19	0.14	0.060	0.74	0.022	13.09	38
2018/3/8	0.18	0.20	0.14	0.15	0.76	0.049	11.49	23
2018/4/2	0.18	0.25	0.11	0.17	0.72	0.058	9.19	19
2018/5/1	0.10	0.17	0.17	0.094	0.68	0.033	14.10	31
2018/6/14	0.12	0.24	0.12	0.057	0.67	0.021	10.92	37
2018/7/12	0.12	0.34	0.08	0.068	0.66	0.025	7.77	29
2018/8/1	0.076	0.21	0.13	0.051	0.67	0.019	12.18	41

Table S.16: Estimation of pharmaceutical attenuation in Muddy Creek and attenuation percentage when Muddy Creek enters Iowa River. Median travel time from WWTP outfall to Iowa River is 37.91 h.

Chemical	Rate constant ± standard error (median, h^{-1})	$C_{Iowa\ River}/C_{Effluent}$ ±standard deviation	Attenuation percentage	Half-life (h)
Atenolol	0.0187 ±0.0040	0.38±0.15	62%	37
Bupropion	0.0554 ±0.0040	0.18±0.20	82%	12
Carbamazepine	0.0291 ±0.0023	0.39±0.23	61%	24
Citalopram	0.219 ±0.0172	0	100%	3
Desvenlafaxine	0.0348 ±0.0022	0.29±0.15	71%	20
Fexofenadine	0.0295 ±0.0008	0.32±0.14	68%	24
Fluconazole	0.0242 ±0.0047	0.45±0.24	55%	29
Guanylurea	0.0172 ±0.0094	0.43±0.20	57%	40
Lidocaine	0.0227 ±0.0036	0.38±0.22	62%	30
Metformin	0.0399 ±0.0038	0.19±0.27	81%	17
Methocarbamol	0.0362 ±0.0175	0.33±0.20	67%	19
Sulfamethoxazole	0.0098 ±0.0039	0.47±0.15	53%	71
Tramadol	0.0283 ±0.0019	0.29±0.15	71%	24
Venlafaxine	0.0451 ±0.0021	0.17±0.11	83%	15

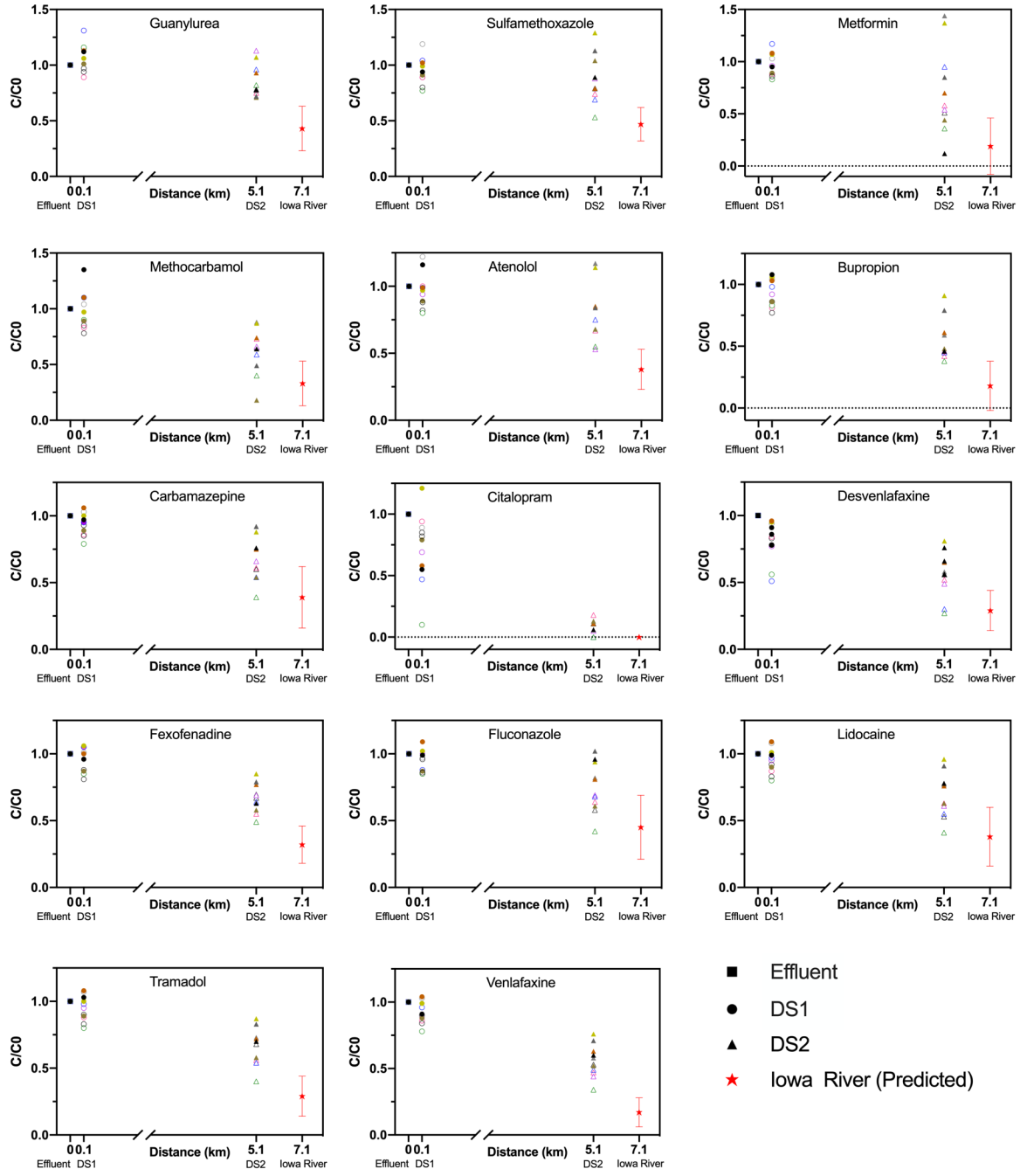

Figure S.11: Measured (Effluent, DS1, DS2 in Muddy Creek, Iowa) and predicted concentrations (Iowa River) of pharmaceuticals and industrial chemicals in the effluent and along the stream reach. The red star with standard error bar is the predicated concentration at the confluence of Muddy Creek and the Iowa River based on the rate constant, it also corresponds the location of the red star in Fig. 1. in the manuscript, whereas other data points at a given location are individual sampling dates measured results during Year 1. The red star is the predicted concentration ratio at the end of the stream reach, at the confluence of Muddy Creek and the Iowa river and corresponds to the location of the red star in Fig. 1. Different shapes represent corresponding sampling locations. Different colors represent different sampling date.

Table S.17: Rate constants ± standard error (unit: h^{-1}) of each monthly sampling set at three sites (effluent, DS1 and DS2) during September 2017 to August 2018.[2]

Chemical	Sep (2017)	Oct (2017)	Nov (2017)	Dec (2017)	Jan (2018)	Feb (2018)	Mar (2018)	Apr (2018)	May (2018)	Jun (2018)	Jul (2018)	Aug (2018)	Median
Atenolol	-1.154*#	0.0132 ±0.0061	0.0187 ±0.0040	0.0112 ±0.0004	NA	-0.0099 ±0.0017#	0.0525 ±0.0137	0.0316 ±0.0005	0.0454 ±0.0026	0.0366 ±0.0003	0.0517 ±0.0169	-0.0125 ±0.0115#	0.0187 ±0.0040
Bupropion	0.0623 ±0.0050	0.0177 ±0.0133	0.0364 ±0.0049	0.0350 ±0.0018	NA	0.0068 ±0.0028	0.0846 ±0.0110	0.0882 ±0.0008	0.0554 ±0.0040	0.0790 ±0.0130	0.1019 ±0.0129	0.0443 ±0.0027	0.0554 ±0.0040
Carbamazepine	0.0219 ±0.0016	0.0060 ±0.0087	0.0300 ±0.0039	0.0203 ±0.0031	NA	0.0099 ±0.0001	0.0829 ±0.0141	0.0675 ±0.0033	0.0291 ±0.0023	0.0459 ±0.0094	0.0657 ±0.0059	0.0065 ±0.0018	0.0291 ±0.0023
Citalopram	0.2256 ±0.0321	0.2020 ±0.0087	0.1018 ±0.0075	0.1538 ±0.0255	NA	0.1694 ±0.0115	0.3715 ±0.1414	0.4917 ±0.0536	0.2187 ±0.0172	0.1594 ±0.0026	0.2846 ±0.0134	0.2316 ±0.0046	0.2187 ±0.0172
Desvenlafaxine	0.0284 ±0.0015	0.0162 ±0.0102	0.0271 ±0.0039	0.0231 ±0.0036	NA	0.0115 ±0.0006	0.0855 ±0.0140	0.0676 ±0.0048	0.0348 ±0.0022	0.0551 ±0.0067	0.0632 ±0.0096	0.0353 ±0.0032	0.0348 ±0.0022
Fexofenadine	0.0381 ±0.0020	0.0177 ±0.0107	0.02271 ±0.0046	0.0189 ±0.0001	NA	0.0122 ±0.0033	0.0620 ±0.0099	0.0489 ±0.0043	0.0255 ±0.0027	0.0551 ±0.0099	0.0517 ±0.0115	0.0295 ±0.0008	0.0295 ±0.0008
Fluconazole	0.0032 ±0.0005	-0.0013 ±0.0077#	0.0242 ±0.0047	0.0153 ±0.0041	NA	0.0053 ±0.0011	0.0768 ±0.0092	0.0426 ±0.0096	0.0255 ±0.0012	0.0414 ±0.0100	0.0708 ±0.0031	0.0164 ±0.0016	0.0242 ±0.0047
Guanylurea	0.0193 ±0.0064	0.0241 ±0.0029	0.0172 ±0.0005	0.0048 ±0.0060	NA	-0.0046#	0.0172 ±0.0094	0.0040 ±0.0208	0.0087 ±0.0135#	0.0258 ±0.0076	0.0322 ±0.0025	0.0220 ±0.0083	0.0172 ±0.0094
Lidocaine	0.0194 ±0.0004	0.0074 ±0.0097	0.0227 ±0.0036	0.0188 ±0.0041	NA	0.0030 ±0.0006	0.0777 ±0.0135	0.0642 ±0.0018	0.0348 ±0.0022	0.0423 ±0.0087	0.0812 ±0.0067	0.0213 ±0.0042	0.0227 ±0.0036
Metformin	0.1693 ±0.0022	0.0125 ±0.0076	0.0399 ±0.0038	0.0252 ±0.0037	NA	-0.0237 ±0.0036#	0.0898 ±0.0109	0.0052 ±0.0124	0.0433 ±0.0016	0.0505 ±0.0074	0.0877 ±0.0103	-0.0304 ±0.0015#	0.0399 ±0.0038
Methocarbamol	0.0362 ±0.0175	0.0527 ±0.0125	0.0855 ±0.0034	0.0209 ±0.0046	NA	0.0107 ±0.0015	0.0793 ±0.0061	0.0564 ±0.0082	0.0299 ±0.0048	0.0295 ±0.0114	0.0556 ±0.0142	0.0106 ±0.0024	0.0362 ±0.0175
Sulfamethoxazole	0.0098 ±0.0039	-0.0086 ±0.0114#	-0.0019 ±0.0031#	0.0161 ±0.0011	NA	-0.0199 ±0.0007#	0.0551 ±0.0155	0.0402 ±0.0034	0.0092 ±0.0021	0.0285 ±0.0069	0.0310 ±0.0098	-0.0100 ±0.0104#	0.0098 ±0.0039
Tramadol	0.0283 ±0.0019	0.0140 ±0.0092	0.0271 ±0.0036	0.0230 ±0.0041	NA	0.0107 ±0.0001	0.0803 ±0.0129	0.0675 ±0.0010	0.0440 ±0.0021	0.0542 ±0.0080	0.0490 ±0.0087	0.0262 ±0.0043	0.0283 ±0.0019
Venlafaxine	0.0422 ±0.0048	0.0249 ±0.0091	0.0325 ±0.0042	0.0322 ±0.0017	NA	0.0214 ±0.0004	0.0934 ±0.0146	0.0773 ±0.0032	0.0575 ±0.0045	0.0697 ±0.0092	0.0812 ±0.0085	0.0451 ±0.0021	0.0451 ±0.0021

Note: NA indicates that the flow rate at DS2 in January was not available due to the water was ice-affected at DS2. * indicates that chemical at DS2 was not detected, thus only two data points (one in the effluent and the other one at DS1) was fitted into the first-order kinetics equation. # indicates higher concentrations were detected in either DS1 or DS2 compared to Effluent.

Table S.18: Human health benchmark concentration (HHBs) of emerging contaminants.[56] For the majority of pharmaceuticals, there are no HHBs applicable/available.

Chemical	Human risk limits (HRLs, µg/L)	Health based values (HBVs, µg/L)	Risk assessment advice (RAA, µg/L)
Atrazine	3	–	–
1H-benzotriazole	–	20	–
5-methyl-1H-benzotriazole	–	–	20
Carbamazepine	40	–	–
Clothianidin	200	–	–
Desvenlafaxine	–	20	–
Imidacloprid	–	3;100	–
Sulfamethoxazole	–	–	100
Thiamethoxam	200;400	–	–
Venlafaxine	–	10	–

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