



Research article

Occurrence and aquatic toxicity of contaminants of emerging concern (CECs) in tributaries of an urbanized section of the Delaware River Watershed

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Table S1. LC retention times and MRM parameters.

Compound	Retention time (min)	Precursor ion (m/z)	Product ion (m/z)	Cone Voltage (V)	Collision Voltage (V)
Carbamazepine	3.41	237.16	165.11	34	42
			179.05	34	44
Clarithromycin	3.38	748.78	116.02	28	64
			158.11	28	40
Diltiazem	3.23	415.34	150.04	16	56
			178.06	16	34
Dehydronifedipine	3.47	345.22	268.11	44	36
			284.19	44	36
Diphenhydramine	3.21	256.22	152.01	14	44
			162.013	14	18
Erythromycin	3.47	734.78	158.11	28	46
			576.66	28	24
Sulfamethoxazole	3.12	254.13	92.05	26	16
Tiabendazole	3.02	202.07	131.09	46	38
			175.03	46	30
Trimethoprim	2.89	291.22	123.06	40	32
			230.16	40	32

Table S2. Sample sites.

Sample Site	Watershed	Agency	Sampling Coordinates		Location
			Latitude	Longitude	
I	North Branch Neshaminy Creek	DRBC	40.288436	-75.203283	Rt 152 Chalfont, PA
J	Neshaminy Creek	DRBC	40.269511	-75.074103	Mill Road West, Jamison PA
H	East Branch of Perkiomen Creek	DRBC	40.357747	-75.307885	North Main Street, Sellersville, PA
G	East Branch of Perkiomen Creek	DRBC	40.343008	-75.336636	Cathill Rd, Telford, PA
D	Perkiomen Creek	DRBC	40.209282	-75.449974	Bridge Rd (Rt 113 near intersection with Rt 29) , Perkiomen, PA
F	Wissahickon Creek	DRBC	40.146801	-75.226237	12 Morris Rd, Ambler, PA
C	Wissahickon Creek	DRBC	40.123833	-75.219861	544 Skippack Pike, Fort Washington Park, Fort Washington, PA
E	Wissahickon Creek	DRBC	40.084336	-75.227702	Germantown Bridge, Germantown Ave, Chestnut Hill, PA
B	Schuylkill River	DRBC	40.0706	-75.3096	Fayette Street Bridge, W. Conshohocken, PA
A	Schuylkill River	DRBC USGS/PADEP	40.00840691	-75.19766536	Falls Bridge, East Falls, Philadelphia, PA

Table S3. In-field measurements.

Sample	Date	Time	Temp (°C)	DO (mg/L)	DO % sat	Specific Conductivity (µS/mL)	pH	Turbidity NTU
EC-C-091113	09/11/13	1010	21.59	6.97	78.9	867.4	6.94	1.48
EC-I-091113	09/11/13	1115	23.16	7.6	88.6	230.2	6.7	4.19
EC-G-091113	09/11/13	1201	23.60	8.88	104.5	346.5	7.97	4.47
EC-E-091713	09/17/13	930	15.47	9.21	92.3	823	8.06	77
EC-F-091713	09/17/13	1030	14.95	9.64	95.8	991.8	7.98	0
EC-J-091713	09/17/13	1115	16.67	9.88	101.8	675.8	8.2	0
EC-H-091713	09/17/13	1212	17.70	8.97	94.3	227	7.83	3.8
EC-D-091713	09/17/13	1336	18.29	10.61	113	375	8.33	3.4
EC-B-091713	09/17/13	1427	20.68	9.76	109.1	529	8.21	4.4
EC-A-091713	09/17/13	1505	20.59	9.29	103.6	567.9	8.11	1.2
EC-E-100313	10/03/13	942	16.89	8.16	84.5	847.8	8.05	1.8
EC-C-100313	10/03/13	1005	17.76	8.9	93.7	907.1	7.77	0
EC-F-100313	10/03/13	1022	17.01	9.1	94.5	1053	7.93	0
EC-J-100313	10/03/13	1109	18.34	8.95	95.6	711.4	8.05	0
EC-I-100313	10/03/13	1130	18.94	8.03	86.5	258.7	7.61	10.8
EC-H-100313	10/03/13	1222	18.93	8.36	90.1	272.8	7.79	2.6
EC-G-100313	10/03/13	1243	19.50	9.86	108.2	404.9	8.08	0.2
EC-D-100313	10/03/13	1404	20.32	10.7	118.6	388.1	8.43	1
EC-B-100313	10/03/13	1448	21.32	9.63	108.9	572.4	8.36	46.6
EC-A-100313	10/03/13	1527	20.36	8.96	99.4	577.6	8.21	0.5
EC-E-042814	04/28/14	900	13.17	8.87	84.6	752.9	7.91	3.96
EC-C-042814	04/28/14	930	12.58	11.46	108	728.5	7.83	2.94
EC-F-042814	04/28/14	1000	14.81	12.02	118.9	679	8.13	1.42
EC-J-042814	04/28/14	1251	15.08	13.73	136.6	583.2	8.73	1.99
EC-I-042814	04/28/14	1355	16.79	11.65	120.2	384	8.34	7.73
EC-H-042814	04/28/14	1425	15.05	10.72	106.3	273.4	8.47	4.41
EC-G-042814	04/28/14	1442	18.08	13.24	140.6	408.6	9.43	2.07
EC-D-042814	04/28/14	1527	16.55	13.58	139	324.6	9	2.33
EC-B-042814	04/28/14	1618	15.96	10.16	103	368.5	7.95	5.47
EC-A-042814	04/28/14	1707	15.52	10.44	104.7	372.6	8.04	5.19

Table S4. Occurrence data.*

Analyte	Sample Set	Sample	Sampling Sites									
			EC-A	EC-B	EC-C	EC-D	EC-E	EC-F	EC-G	EC-H	EC-I	EC-J
Clarithromycin	1	1	3.4	6	0.1	0.8	11.2	14.8	4.8	0.8	15.6	2
	1	2	0.5	7	0.1	1.2	11.1	5.2	6.9	0.9	13.9	3.7
	2	1	4.6	6	10.8	1.6	8.5	6.6	3.4	0.8	0.2	2.6
	2	2	5.8	5.7	11.4	1.6	8.4	6.9	5.1	0.3	0.2	3.7
	3	1	1.7	2.1	5.5	ND	5.6	3.5	5.6	ND	ND	5.1
	3	2	2.2	2.2	6.1	1	5.3	2.8	4.5	ND	ND	5.7
Trimethoprim	1	1	11.8	21.6	7.3	0.4	26	0.9	11.7	5.4	63.2	9.9
	1	2	9.2	32.7	7.9	1.5	24	0.8	10.4	12.5	48.1	17.6
	2	1	4.2	7.1	14.7	0.2	6.6	0.5	4.9	0.8	1	3.8
	2	2	5.6	23.7	15.8	0.2	6.3	0.4	6.4	0.5	0.1	3.7
	3	1	6	6.4	19.1	ND	16	ND	20.7	ND	14.7	14
	3	2	6.3	8.2	19.8	ND	16.4	ND	15.9	ND	11.6	ND
Carbamazepine	1	1	71.5	62.1	40.9	63.1	112.9	138.9	133	NA	176.9	132.7
	1	2	74.5	58.6	45.9	60.7	129.4	118.4	140	NA	176	141.8
	2	1	128.1	125.4	243	120.2	190.7	183.4	143	78.4	73	208.2
	2	2	119.2	114.2	242.8	113.9	186.2	177.3	145.5	73.3	83.1	203.6
	3	1	11.6	11.4	34.3	34.9	27.4	15.7	118.5	3	2.3	25.3
	3	2	10.2	11.7	39.9	47.4	30.5	13.3	110.6	3.6	3.4	23
Diphenhydramine	1	1	8.3	8.2	3.7	2.4	11.5	4	3.3	1.6	38.6	4
	1	2	14.4	8	4.8	0.6	10.4	NA	1.9	NA	37	4.1
	2	1	24.4	44.6	57.5	2.1	11.5	NA	13.1	0.8	2.7	NA
	2	2	36.7	28.8	101	NA	23.9	4	21.1	2.5	2.5	NA
	3	1	5.8	9.8	8.7	1.9	8.9	5	57.7	ND	1.8	6.3
	3	2	8.2	7.6	12	1.9	10.7	5.7	55.7	2	1	8.5
Dehydronifedipine	1	1	1.3	1.3	NA	0.5	3.6	6.7	0.8	NA	6.2	4.1
	1	2	0.8	1.4	0.4	0.7	4.6	3.4	1	NA	8	6
	2	1	1.9	2.3	8.6	1.2	4.6	6.7	2.1	0.6	0.7	7.5
	2	2	2.1	1.6	8.4	1.2	4.7	5.8	1.3	0.6	0.3	6.7
	3	1	8.2	1.6	3.5	3	2.3	1.7	1.8	ND	ND	8.1
	3	2	2	ND	3.6	5.9	2.5	6.8	1	4.2	4.7	2.4
Diltiazem	1	1	NA	0.9	NA	NA	2.2	0.4	NA	NA	6.6	0.5
	1	2	0.4	0.8	NA	NA	3.2	0.6	NA	NA	8	1.5
	2	1	1.4	1.2	4.5	0.5	1.5	0.9	2.4	0.4	0.4	2
	2	2	1.1	0.8	4.5	0.9	2.5	1.1	2.7	0.00	0.5	1.8
	3	1	1.3	2.2	7.4	ND	6.6	2.8	2.9	ND	ND	2.2
	3	2	2.9	1.8	8.2	ND	6.5	3.1	1.4	ND	ND	2.6

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Analyte	Sample Set	Sample	Sampling Sites									
			EC-A	EC-B	EC-C	EC-D	EC-E	EC-F	EC-G	EC-H	EC-I	EC-J
Erythromycin	1	1	NA	23.5	NA	NA	52.1	NA	7.5	0.5	56.1	1.6
	1	2	1.5	21.3	1	6.4	55.6	NA	10.7	0.8	57.7	NA
	2	1	0.6	28.4	NA	NA	NA	NA	NA	NA	NA	NA
	2	2	NA	27.6	NA	NA	NA	NA	NA	3.4	0.2	NA
	3	1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	3	2	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
Gemfibrozil	1	1	13.5	23.9	0.5	2.7	18.2	NA	1.3	0.4	26.8	2.4
	1	2	11.2	21.3	NA	2.7	17.9	NA	0.7	0.6	20.8	1.9
	2	1	18.4	21.2	30.5	1	13.9	0.8	5.5	3.2	0.8	3.5
	2	2	21.1	25.4	32.6	0.6	13.7	0.6	4.5	3.7	0.2	3.4
	3	1	12	13.8	9.6	6.8	8	4	93	1.4	1.3	10.1
	3	2	13.4	14.4	10.3	7.4	8.5	3.7	70.8	2	1.2	10.5
Ibuprofen	1	1	99.5	151.7	4.7	13.9	18.1	7.3	6.1	16.1	28.3	62.9
	1	2	90.3	40	29.3	8	15.1	18.2	3.7	5.9	3.8	7.5
	2	1	38.3	34.2	32.2	5.2	15	NA	11.6	6.5	NA	30.1
	2	2	40.1	26	32.4	9.9	17.9	12.6	9.6	5.9	4.2	20.9
	3	1	33.9	35.6	29.7	9.2	29	33.2	26.9	6.8	22.7	27.8
	3	2	32.1	27.5	48.1	12.4	32.3	17.5	26.6	5.5	18.7	25.6
Triclocarban	1	1	9.3	15.2	37.6	265.1	18.5	18.7	69.2	196.6	6.3	52
	1	2	10.5	30.8	38.7	108.2	71.8	11.7	35.7	120	35.8	63.7
	2	1	55.3	59.5	95.2	76.6	48.1	45.3	74.5	68.1	82	42.4
	2	2	87.7	22.3	52.5	84.6	47.9	87.4	53.7	89.9	79.6	44.1
	3	1	30.3	32	34	33.8	25.9	22.9	18.2	35.1	34.9	26.7
	3	2	27.5	29.7	26.6	24.2	26.9	35.4	39.3	27.5	31.9	30.7
Metformin	1	1	4354	933	4370	1804	3536	2646	2747	1008	1066	3576
	1	2	3819	959	4316	1944	3708	2486	2840	1076	994	4349
	2	1	4056	5848	9242	NA	4207	4459	4193	NA	NA	7514
	2	2	4851	4447	9258	NA	4223	4406	4024	NA	NA	7672
	3	1	NA	NA	3095	3403	2955	2114	6507	1271	1009	3551
	3	2	NA	4642	3308	NA	3290	2181	6007	1141	1131	3640
Ranitidine	1	1	1.8	4.1	86.4	0.8	42.7	1.6	8.7	NA	0.1	9.1
	1	2	1.9	3.4	90.4	NA	48.3	2	8.5	0.5	NA	11.7
	2	1	1.7	1.9	106	0.6	23.3	1.1	17	0.1	NA	8.7
	2	2	2.4	1.8	72.1	0.7	18.9	NA	14.8	0.1	NA	10.8
	3	1	5.5	11.7	83	2.2	42.5	5.3	70.3	1.3	ND	12.5
	3	2	5.1	9.7	83.3	3	50.6	6.2	71.5	1	NA	12.9

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Analyte	Sample Set	Sample	Sampling Sites									
			EC-A	EC-B	EC-C	EC-D	EC-E	EC-F	EC-G	EC-H	EC-I	EC-J
Sulfamethoxazole	1	1	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	1	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	2	1	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	2	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	3	1	3.9	5.3	24	3.6	19.8	5.8	7.1	1	ND	12.7
	3	2	5.1	5.4	24	5.8	21.1	4.2	8.6	1.2	ND	12.1
Thiabendazole	1	1	11	7.8	2.3	0.2	71.9	190.7	4.1	0.5	134.9	12.7
	1	2	4.6	14.2	0.5	3.5	87.8	150.2	4.5	2.5	113.1	11.5
	2	1	12.2	11	73.9	6	49.3	173.2	10.7	0.1	2.9	13.2
	2	2	15.8	11.1	74	5	59.6	155.9	10.3	1.1	3.6	17.9
	3	1	4	3.3	26	1.9	5.2	13.3	4.6	4.6	1.1	ND
	3	2	ND	2.7	5.7	1.3	5.5	12.5	1.8	6.1	1	2.1
Guanylurea	1	1	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	1	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	2	1	130.7	158.9	620.1	NA	299.3	49.9	352.5	NA	NA	139.3
	2	2	127.2	173.7	458.5	33.7	168.7	NA	311.8	12.3	NA	144.9
	3	1	12	10.6	44	11.8	34.3	20.9	82.6	2.9	ND	31.6
	3	2	10.2	12	45.7	10	58.3	25.5	95.6	6.4	NA	36.5

*Notes: Sample set 1 was on 09/11/13-09/17/13; Sample set 2 was on 10/03/13; Sample set 3 was on 04/28/14; ND – non-detect; NA – not available.



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