

## Supporting Information

**Title:** Occurrence of antibiotics, estrogenic hormones, and UV-filters in water, sediment, and oyster tissue from the Chesapeake Bay

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**Table S1. Salient information for the target antibiotics, estrogenic hormones, UV-filters, and the corresponding isotopically-labeled internal standards.**

Chemical	Acronym	Formula	pK <sub>a</sub> values	log D (pH 7) <sup>a</sup>
<b>Fluoroquinolones</b>				
Ciprofloxacin	CIP	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	6.3; 8.8 <sup>b</sup>	-0.81
Ciprofloxacin-d <sub>8</sub>	CIP-d <sub>8</sub>	C <sub>17</sub> H <sub>10</sub> D <sub>8</sub> FN <sub>3</sub> O <sub>3</sub>	-	-
Difloxacin	DIF	C <sub>21</sub> H <sub>19</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	5.8; 8.3 <sup>b</sup>	1.96
Difloxacin-d <sub>3</sub>	DIF-d <sub>3</sub>	C <sub>21</sub> H <sub>16</sub> D <sub>3</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	-	-
Enoxacin	ENO	C <sub>15</sub> H <sub>17</sub> FN <sub>4</sub> O <sub>3</sub>	5.5; 8.6 <sup>c</sup>	-0.98
Enrofloxacin	ENR	C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>3</sub>	6.1; 7.9 <sup>b</sup>	0.89
Fleroxacin	FLE	C <sub>17</sub> H <sub>18</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	5.4; 6.1 <sup>a</sup>	0.47
Gatifloxacin	GAT	C <sub>19</sub> H <sub>22</sub> FN <sub>3</sub> O <sub>4</sub>	5.7; 8.7 <sup>a</sup>	-0.58
Lomefloxacin	LOM	C <sub>17</sub> H <sub>19</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	5.8; 9.3 <sup>c</sup>	-0.39
Marbofloxacin	MAR	C <sub>17</sub> H <sub>19</sub> FN <sub>4</sub> O <sub>4</sub>	5.5; 8.4 <sup>b</sup>	-0.65
Moxifloxacin	MOX	C <sub>21</sub> H <sub>24</sub> FN <sub>3</sub> O <sub>4</sub>	5.4; 6.2 <sup>a</sup>	-0.50
Nadifloxacin	NAD	C <sub>19</sub> H <sub>21</sub> FN <sub>2</sub> O <sub>4</sub>	6.1 <sup>a</sup>	0.92
Norfloxacin	NOR	C <sub>16</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	6.3; 8.4 <sup>b</sup>	-0.92
Ofloxacin	OFL	C <sub>18</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>4</sub>	5.5; 6.2 <sup>a</sup>	0.07
Ofloxacin-d <sub>3</sub>	OFL-d <sub>3</sub>	C <sub>18</sub> H <sub>17</sub> D <sub>3</sub> FN <sub>3</sub> O <sub>4</sub>	-	-
Orbifloxacin	ORB	C <sub>19</sub> H <sub>20</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	5.5; 8.8 <sup>a</sup>	0.25
Pefloxacin	PEF	C <sub>17</sub> H <sub>20</sub> FN <sub>3</sub> O <sub>3</sub>	5.7; 6.5 <sup>a</sup>	0.49
Sarafloxacin	SAR	C <sub>20</sub> H <sub>17</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	5.9; 8.9 <sup>c</sup>	0.56
Sparfloxacin	SPA	C <sub>19</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	5.8; 8.8 <sup>a</sup>	-0.04
Tosufloxacin	TOS	C <sub>19</sub> H <sub>15</sub> F <sub>3</sub> N <sub>4</sub> O <sub>3</sub>	5.4; 9.6 <sup>a</sup>	0.47
<b>Macrolides</b>				
Azithromycin	AZI	C <sub>38</sub> H <sub>72</sub> N <sub>2</sub> O <sub>12</sub>	8.9; 9.6 <sup>a</sup>	-1.99
Azithromycin-d <sub>3</sub>	AZI-d <sub>3</sub>	C <sub>38</sub> H <sub>69</sub> D <sub>3</sub> N <sub>2</sub> O <sub>12</sub>	-	-
Clarithromycin	CLA	C <sub>38</sub> H <sub>69</sub> NO <sub>13</sub>	8.4 <sup>a</sup>	1.84
Erythromycin	ERY	C <sub>37</sub> H <sub>67</sub> NO <sub>13</sub>	8.4 <sup>a</sup>	1.20
Erythromycin-d <sub>6</sub>	ERY-d <sub>6</sub>	C <sub>37</sub> H <sub>61</sub> D <sub>6</sub> NO <sub>13</sub>	-	-
Roxithromycin	ROX	C <sub>41</sub> H <sub>76</sub> N <sub>2</sub> O <sub>15</sub>	2.3; 9.1 <sup>a</sup>	0.93
Tylosin	TYL	C <sub>46</sub> H <sub>77</sub> NO <sub>17</sub>	7.2 <sup>a</sup>	1.91
<b>Sulfonamides</b>				
Sulfacetamide	SCM	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	2.1; 4.3 <sup>a</sup>	-1.20
Sulfadiazine	SDZ	C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S	2.0; 7.0 <sup>a</sup>	0.13
Sulfadimethoxine	SDM	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S	2.1; 6.1 <sup>c</sup>	0.97
Sulfadoxine	SDX	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>4</sub> S	2.6; 6.1 <sup>a</sup>	-0.08
Sulfamerazine	SMR	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S	2.1; 6.9 <sup>c</sup>	0.26
Sulfadimidine	SDD	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	2.1; 7.5 <sup>c</sup>	0.39
Sulfamethizole	SMZ	C <sub>9</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	1.9; 5.3 <sup>c</sup>	-0.17
Sulfamethizole- <sup>13</sup> C <sub>6</sub>	SMZ- <sup>13</sup> C <sub>6</sub>	<sup>13</sup> C <sub>6</sub> C <sub>3</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	-	-
Sulfamethoxazole	SMX	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S	1.7; 5.6 <sup>c</sup>	0.14
Sulfamethoxazole- <sup>13</sup> C <sub>6</sub>	SMX- <sup>13</sup> C <sub>6</sub>	<sup>13</sup> C <sub>6</sub> C <sub>4</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> S	-	-
Sulfaphenazole	SPZ	C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	2.0; 2.7; 6.9; <sup>a</sup>	1.51
Sulfapyridine	SPD	C <sub>11</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S	2.1; 6.2 <sup>a</sup>	0.40
Sulfaquinoxaline	SQX	C <sub>14</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S	1.9; 5.5 <sup>c</sup>	1.21
Sulfaquinoxaline- <sup>13</sup> C <sub>6</sub>	SQX- <sup>13</sup> C <sub>6</sub>	<sup>13</sup> C <sub>6</sub> C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub> S	-	-
Sulfathiazole	STZ	C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>	2.0; 7.1 <sup>c</sup>	0.69
Sulfisomidine	SSD	C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	2.0; 5.0; 6.1 <sup>a</sup>	0.44
<b>Tetracyclines</b>				
Chlortetracycline	CTC	C <sub>22</sub> H <sub>23</sub> ClN <sub>2</sub> O <sub>8</sub>	3.3; 7.6; 9.3 <sup>c</sup>	-3.09
Demeclocycline	DMC	C <sub>21</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>8</sub>	3.4; 7.4; 9.4 <sup>c</sup>	-3.38
Doxycycline	DC	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>	3.0; 8.0; 9.2 <sup>c</sup>	-3.41
Meclocycline	MC	C <sub>22</sub> H <sub>21</sub> ClN <sub>2</sub> O <sub>8</sub>	4.1; 6.9; 9.6 <sup>c</sup>	-4.29

Chemical	Acronym	Formula	pK <sub>a</sub> values	log D (pH 7) <sup>a</sup>
Methacycline	MTC	C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>8</sub>	3.0; 7.3; 9.0 <sup>d</sup>	-3.64
Oxytetracycline	OTC	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub>	3.2; 7.5; 8.9 <sup>c</sup>	-4.64
Rolitetracycline	RTC	C <sub>27</sub> H <sub>33</sub> N <sub>3</sub> O <sub>8</sub>	3.2; 7.4; 8.9 <sup>a</sup>	-2.81
Tetracycline	TC	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>	3.3; 7.8; 9.6 <sup>c</sup>	-3.57
Tetracycline-d <sub>6</sub>	TC-d <sub>6</sub>	C <sub>22</sub> H <sub>18</sub> D <sub>6</sub> N <sub>2</sub> O <sub>8</sub>	-	-
<b><i>Estrogenic hormones</i></b>				
17 $\alpha$ -ethynylestradiol	EE2	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>	10.3 <sup>a</sup>	3.90
17 $\alpha$ -ethynylestradiol-2,4,16,16-d <sub>4</sub>	EE2-d <sub>4</sub>	C <sub>20</sub> D <sub>4</sub> H <sub>20</sub> O <sub>2</sub>	-	-
17 $\beta$ -estradiol	E2	C <sub>18</sub> H <sub>24</sub> O <sub>2</sub>	10.3 <sup>a</sup>	3.75
17 $\beta$ -estradiol-16,16,17-d <sub>3</sub>	E2-d <sub>3</sub>	C <sub>18</sub> D <sub>3</sub> H <sub>21</sub> O <sub>2</sub>	-	-
Estrone	E1	C <sub>18</sub> H <sub>22</sub> O <sub>2</sub>	10.3 <sup>a</sup>	4.31
<b><i>UV-filters</i></b>				
2-ethylhexyl 4-methoxycinnamate	EHMC	C <sub>18</sub> H <sub>26</sub> O <sub>3</sub>	-	5.38
2-ethyl-d5-hexyl-2,3,3,4,4,5,5,6,6,6-d10 4-methoxycinnamate	EHMC-d <sub>15</sub>	C <sub>18</sub> D <sub>15</sub> H <sub>11</sub> O <sub>3</sub>	-	-
4-methylbenzylidene camphor	4-MBC	C <sub>18</sub> H <sub>22</sub> O	-	5.12
4-methyl-benzylidene-d <sub>4</sub> camphor	4-MBC-d <sub>4</sub>	C <sub>18</sub> D <sub>4</sub> H <sub>18</sub> O	-	-
Benzophenone-3	BP-3	C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>	7.1 <sup>a</sup>	3.36
Benzophenone-3-(phenyl-d5)	BP-3-d <sub>5</sub>	C <sub>14</sub> D <sub>5</sub> H <sub>7</sub> O <sub>3</sub>	-	-
Homosalate	HMS	C <sub>16</sub> H <sub>22</sub> O <sub>3</sub>	9.7 <sup>a</sup>	5.00
Homosalate-(benzoic ring-d4)	HMS-d <sub>4</sub>	C <sub>16</sub> D <sub>4</sub> H <sub>18</sub> O <sub>3</sub>	-	-
Octocrylene	OC	C <sub>24</sub> H <sub>27</sub> NO <sub>2</sub>	-	6.78
Octocrylene-(2-ethyl-d5-hexyl-2,3,3,4,4,5,5,6,6,6-d10)	OC-d <sub>15</sub>	C <sub>24</sub> D <sub>15</sub> H <sub>12</sub> NO <sub>2</sub>	-	-

a: values estimated using MarvinSketch v.16.4.25

b: from Jiménez-Lozano *et al.*, 2002 <sup>1</sup>

c: from Qiang and Adams, 2004 <sup>2</sup>

d: from Tam, 2001 <sup>3</sup>

**Table S2. GPS coordinates, water quality, and sampling scheme for the 14 Chesapeake Bay sites investigated in this study.**

Location <sup>a</sup>	Date	Latitude	Longitude	Temp. (°C)	Salinity (ppt)	Water depth (ft)	Water sample	Sediment sample	Oyster sample	Mussel sample
CR-1	6/14/2016	39°00'10.00"N	76°11'51.00"W	n.m. <sup>b</sup>	n.m.	n.m.	+ <sup>c</sup>	- <sup>d</sup>	+	+
CR-2	6/14/2016	39°05'06.00"N	76°09'49.00"W	n.m.	n.m.	n.m.	+	-	+	+
HS-1	4/18/2017	38°07'01.20"N	76°04'23.10"W	18.1	13.0	4.5	+	+	+	-
HS-2	4/18/2017	38°07'00.90"N	76°04'24.30"W	18.0	13.1	5.0	+	+	+	-
HS-3	4/18/2017	38°07'00.60"N	76°04'25.80"W	18.2	13.0	3.5	+	+	+	-
KC-1	4/18/2017	37°58'10.74"N	75°42'05.40"W	19.4	14.8	7.0	+	+	+	-
KC-2	4/18/2017	37°58'05.76"N	75°42'00.06"W	19.2	14.7	6.5	+	+	+	-
KC-3	4/18/2017	37°58'27.00"N	75°42'36.00"W	19.4	15.0	6.5	+	+	+	-
MA-1	4/27/2017	38°08'24.12"N	75°49'29.52"W	17.1	13.9	5.0	+	+	+	-
MA-2	4/27/2017	38°08'09.96"N	75°48'28.86"W	17.2	13.6	6.5	+	+	+	-
MA-3	4/27/2017	38°07'24.06"N	75°51'54.60"W	17.2	15.6	11.0	+	+	+	-
MB-1	4/27/2017	38°07'23.10"N	75°54'51.00"W	17.8	15.7	10.0	+	+	+	-
MB-2	4/27/2017	38°07'04.02"N	75°55'25.38"W	18.1	15.5	9.0	+	+	+	-
MB-3	4/27/2017	38°06'55.90"N	75°55'16.56"W	18.1	15.5	10.0	+	+	+	-

a: CR, Chester River; HS, Holland Straits; KC, Kitts Creek; MA, Manokin River A; MB, Manokin River B; the number refers to distinct sites in each sampling area

b: n.m. indicates that the parameter was not measured at this site

c: + indicates that the sample was collected

d: - indicates that the sample was not collected

**Table S3. ESI-MS/MS operational parameters for antibiotics, estrogenic hormones, UV-filters, and the isotopically-labelled internal standards.**

Chemical	MW <sup>a</sup>	Parent ion	TLO <sup>b</sup>	Fragment ion 1 <sup>c</sup>	CE-1 (V) <sup>d</sup>	Fragment ion 2 <sup>c</sup>	CE-2 (V) <sup>d</sup>	RT <sup>e</sup> (min)	MDL <sup>f</sup> (ng/L)	MQL <sup>g</sup> (ng/L)	IS <sup>h</sup>
<b><i>Fluoroquinolones</i></b>											
Ciprofloxacin	331.4	332.2	75	314.1	20	231.0	36	3.18	0.9	3.0	CIP-d <sub>8</sub>
Ciprofloxacin-d <sub>8</sub>	339.4	340.2	82	322.1	21	235.0	38	3.18	-	-	-
Difloxacin <sup>i</sup>	399.4	400.2	84	382.1	21	356.1	18	4.13	0.6	2.0	DIF-d <sub>3</sub>
Difloxacin-d <sub>3</sub>	402.4	403.2	84	385.1	23	359.1	18	4.13	-	-	-
Enoxacin	320.3	321.2	68	303.1	21	232.0	34	2.64	1.5	5.0	OFL-d <sub>3</sub>
Enrofloxacin <sup>i</sup>	359.4	360.2	82	342.1	20	316.1	17	3.46	0.6	2.0	CIP-d <sub>8</sub>
Fleroxacin	369.3	370.2	92	326.1	16	269.0	24	2.32	0.6	2.0	OFL-d <sub>3</sub>
Gatifloxacin	375.4	376.2	84	358.1	19	261.0	31	5.83	1.5	5.0	DIF-d <sub>3</sub>
Lomefloxacin	351.4	352.2	83	265.1	22	308.1	15	3.70	0.9	3.0	CIP-d <sub>8</sub>
Marbofloxacin <sup>i</sup>	362.4	363.2	83	72.2	22	320.0	12	2.13	1.5	5.0	OFL-d <sub>3</sub>
Moxifloxacin	401.4	402.2	87	384.1	20	364.1	25	8.65	1.5	5.0	DIF-d <sub>3</sub>
Nadifloxacin	360.4	361.2	85	343.1	22	283.0	35	12.12	0.3	1.0	DIF-d <sub>3</sub>
Norfloxacin	319.3	320.2	67	302.2	20	231.0	38	2.93	0.9	3.0	CIP-d <sub>8</sub>
Ofloxacin	361.4	362.2	91	318.1	17	261.0	26	2.56	0.6	2.0	OFL-d <sub>3</sub>
Ofloxacin-d <sub>3</sub>	364.4	365.2	88	321.1	18	261.0	27	2.57	-	-	-
Orbifloxacin <sup>i</sup>	395.4	396.2	86	378.1	19	352.1	16	4.04	0.6	2.0	CIP-d <sub>8</sub>
Pefloxacin	333.4	334.2	83	316.1	20	290.1	17	2.66	0.9	3.0	CIP-d <sub>8</sub>
Sarafloxacin <sup>i</sup>	385.4	386.2	80	368.1	21	299.1	25	4.65	1.5	5.0	DIF-d <sub>3</sub>
Sparfloxacin	392.4	393.2	92	349.1	18	292.1	23	7.92	0.6	2.0	DIF-d <sub>3</sub>
Tosufloxacin	404.4	405.2	79	387.1	23	263.0	45	8.82	0.6	2.0	DIF-d <sub>3</sub>
<b><i>Macrolides</i></b>											
Azithromycin	749.0	375.3	70	591.4	13	158.1	22	8.80	0.1	0.3	AZI-d <sub>3</sub>
Azithromycin-d <sub>3</sub>	752.0	376.8	73	594.4	13	158.1	22	8.81	-	-	-
Clarithromycin	748.0	748.5	102	590.4	16	158.1	26	10.80	0.1	0.3	AZI-d <sub>3</sub>
Erythromycin	733.9	716.5	105	558.4	17	158.1	26	10.77	0.3	1.0	ERY-d <sub>6</sub>
Erythromycin-d <sub>6</sub>	740.0	740.5	99	582.4	17	164.1	29	10.11	-	-	-
Roxithromycin	836.5	837.6	103	679.4	19	158.1	31	10.89	0.3	1.0	ERY-d <sub>6</sub>
Tylosin <sup>i</sup>	916.1	916.6	139	772.5	27	174.1	35	10.12	0.6	2.0	ERY-d <sub>6</sub>
<b><i>Sulfonamides</i></b>											
Sulfacetamide	214.2	215.1	64	156.0	10	92.1	23	2.38	1.5	5.0	SMZ- <sup>13</sup> C <sub>6</sub>
Sulfadiazine	250.3	251.1	68	156.0	15	108.1	23	2.57	1.5	5.0	SMZ- <sup>13</sup> C <sub>6</sub>
Sulfadimethoxine <sup>i</sup>	310.3	311.1	81	156.0	20	173.0	29	8.58	0.3	1.0	SQX- <sup>13</sup> C <sub>6</sub>

Chemical	MW <sup>a</sup>	Parent ion	TLO <sup>b</sup>	Fragment ion 1 <sup>c</sup>	CE-1 (V) <sup>d</sup>	Fragment ion 2 <sup>c</sup>	CE-2 (V) <sup>d</sup>	RT <sup>e</sup> (min)	MDL <sup>f</sup> (ng/L)	MQL <sup>g</sup> (ng/L)	IS <sup>h</sup>
Sulfadoxine	310.3	311.1	79	156.0	17	108.1	27	9.91	0.3	1.0	SQX- <sup>13</sup> C <sub>6</sub>
Sulfamerazine <sup>i</sup>	264.3	265.1	72	156.0	16	108.1	25	3.53	1.5	5.0	SMX- <sup>13</sup> C <sub>6</sub>
Sulfadimidine <sup>i</sup>	278.3	279.1	73	186.0	17	204.0	9	4.90	0.9	3.0	SMX- <sup>13</sup> C <sub>6</sub>
Sulfamethizole	270.3	271.1	72	156.0	13	108.1	23	4.80	1.5	5.0	SMZ- <sup>13</sup> C <sub>6</sub>
Sulfamethizole- <sup>13</sup> C <sub>6</sub>	276.3	277.1	75	162.0	13	114.1	23	4.81	-	-	-
Sulfamethoxazole	253.3	254.1	74	156.0	16	108.1	23	7.75	1.5	5.0	SMX- <sup>13</sup> C <sub>6</sub>
Sulfamethoxazole- <sup>13</sup> C <sub>6</sub>	259.2	260.1	73	162.0	15	114.1	24	7.73	-	-	-
Sulfaphenazole	314.4	315.2	83	222.0	19	158.1	27	9.67	0.6	2.0	SQX- <sup>13</sup> C <sub>6</sub>
Sulfapyridine	249.3	250.1	69	184.0	17	156.0	16	3.08	0.9	3.0	SMX- <sup>13</sup> C <sub>6</sub>
Sulfaquinoxaline <sup>i</sup>	300.4	301.1	75	156.0	15	108.1	27	10.11	0.9	3.0	SQX- <sup>13</sup> C <sub>6</sub>
Sulfaquinoxaline- <sup>13</sup> C <sub>6</sub>	306.3	307.1	74	162.0	16	114.1	27	10.12	-	-	-
Sulfathiazole <sup>i</sup>	255.3	256.1	74	156.0	14	108.1	23	2.76	0.9	3.0	SMX- <sup>13</sup> C <sub>6</sub>
Sulfisomidine	278.3	279.1	80	186.0	15	156.0	19	2.12	0.9	3.0	SMZ- <sup>13</sup> C <sub>6</sub>
<b>Tetracyclines</b>											
Chlortetracycline <sup>i</sup>	478.9	479.2	77	462.1	15	444.1	21	10.13	3.0	10.0	TC-d <sub>6</sub>
Demeclocycline	464.3	465.2	84	448.1	15	430.1	20	5.24	3.0	10.0	TC-d <sub>6</sub>
Doxycycline <sup>i</sup>	444.4	445.2	83	428.1	18	321.0	30	9.58	1.5	5.0	TC-d <sub>6</sub>
Meclocycline	476.9	477.2	86	460.1	19	234.9	35	10.09	1.5	5.0	TC-d <sub>6</sub>
Methacycline	442.4	443.2	81	426.1	16	381.0	22	9.33	1.5	5.0	TC-d <sub>6</sub>
Oxytetracycline <sup>i</sup>	460.4	461.2	90	443.1	12	426.1	19	3.96	3.0	10.0	TC-d <sub>6</sub>
Rolitetra-cycline	527.6	445.2	79	427.1	12	410.1	19	9.58	1.5	5.0	TC-d <sub>6</sub>
Tetracycline <sup>i</sup>	444.4	445.2	79	427.1	13	410.1	19	3.44	3.0	10.0	TC-d <sub>6</sub>
Tetracycline-d <sub>6</sub>	450.5	451.2	81	433.1	11	416.1	19	3.46	-	-	-
<b>Estrogenic hormones</b>											
17 $\alpha$ -ethinylestradiol	296.4	295.1	-105	145.1	-41	159.1	-37	4.92	3.0	10.0	EE2-d <sub>4</sub>
17 $\alpha$ -ethynylestradiol-2,4,16,16-d <sub>4</sub>	300.4	299.1	-111	147.0	-46	161.0	-39	4.93	-	-	-
17 $\beta$ -estradiol	272.4	271.1	-104	183.0	-44	145.1	-42	5.03	1.5	5.0	E2-d <sub>3</sub>
17 $\beta$ -estradiol-16,16,17-d <sub>3</sub>	275.4	274.2	-109	185.1	-45	145.1	-43	5.05	-	-	-
Estrone	270.4	269.1	-106	145.0	-40	143.0	-58	5.14	0.6	2.0	E2-d <sub>3</sub>
<b>UV-filters</b>											
2-ethylhexyl 4-methoxycinnamate	290.4	291.2	68	161.1	18	179.0	5	12.02	0.6	2.0	EHMC-d <sub>15</sub>
2-ethyl-d5-hexyl-2,3,3,4,4,5,5,6,6,6-d <sub>10</sub> 4-methoxycinnamate	305.4	306.3	64	161.1	20	181.1	7	12.03	-	-	-
4-methylbenzylidene camphor	254.4	255.1	87	105.2	31	212.1	17	11.02	0.6	2.0	4-MBC-d <sub>4</sub>
4-methylbenzylidene-d <sub>4</sub> camphor	258.4	259.2	78	109.1	31	216.2	17	11.03	-	-	-
Benzophenone-3	228.2	229.1	73	151.1	19	105.1	19	7.49	0.6	2.0	BP-3-d <sub>5</sub>
Benzophenone-3-(phenyl-d <sub>5</sub> )	233.2	234.2	72	151.1	20	105.1	20	7.52	-	-	-

Chemical	MW <sup>a</sup>	Parent ion	TLO <sup>b</sup>	Fragment ion 1 <sup>c</sup>	CE-1 (V) <sup>d</sup>	Fragment ion 2 <sup>c</sup>	CE-2 (V) <sup>d</sup>	RT <sup>e</sup> (min)	MDL <sup>f</sup> (ng/L)	MQL <sup>g</sup> (ng/L)	IS <sup>h</sup>
Homosalate	262.4	261.1	-78	137.0	-20	93.1	-38	12.58	4.5	15.0	HMS-d <sub>4</sub>
Homosalate-(benzoic ring-d <sub>4</sub> )	266.4	265.1	-77	141.0	-21	97.1	-37	12.60	-	-	-
Octocrylene	361.5	362.2	90	232.0	19	250.2	7	11.52	0.6	2.0	OC-d <sub>15</sub>
Octocrylene-(2-ethyl-d <sub>5</sub> -hexyl-2,3,3,4,4,5,5,6,6,6-d <sub>10</sub> )	376.5	377.3	94	233.1	22	251.1	11	11.55	-	-	-

a: MW, molecular weight (g/mol)

b: TLO, tube lens offset

c: The first fragment ion (Fragment ion 1) was used for quantitation; the second fragment ion (Fragment ion 2) was used for confirmation

d: CE, collision energy

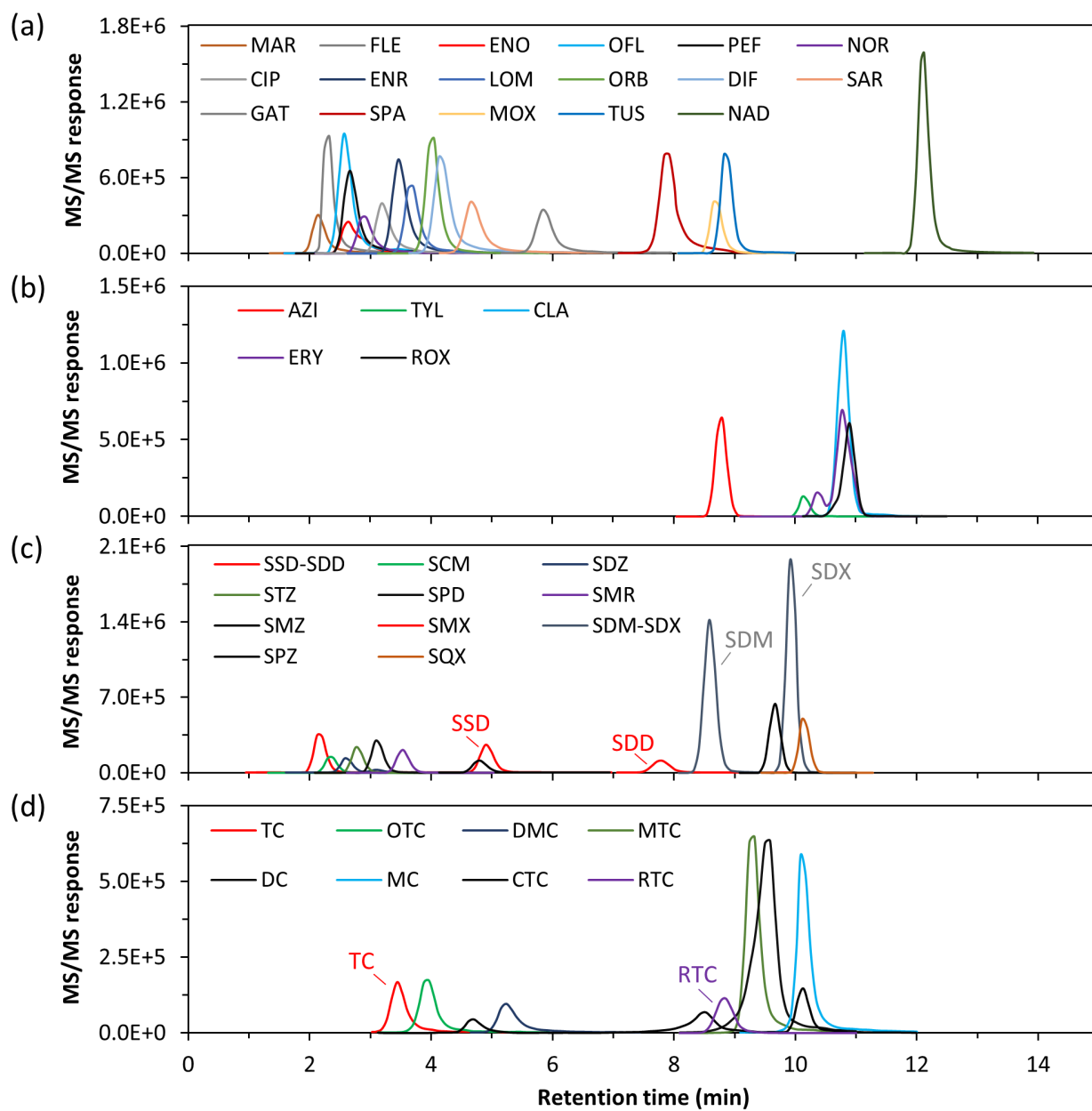
e: RT, retention time

f: MDL, method detection limit

g: MQL, method quantitation limit

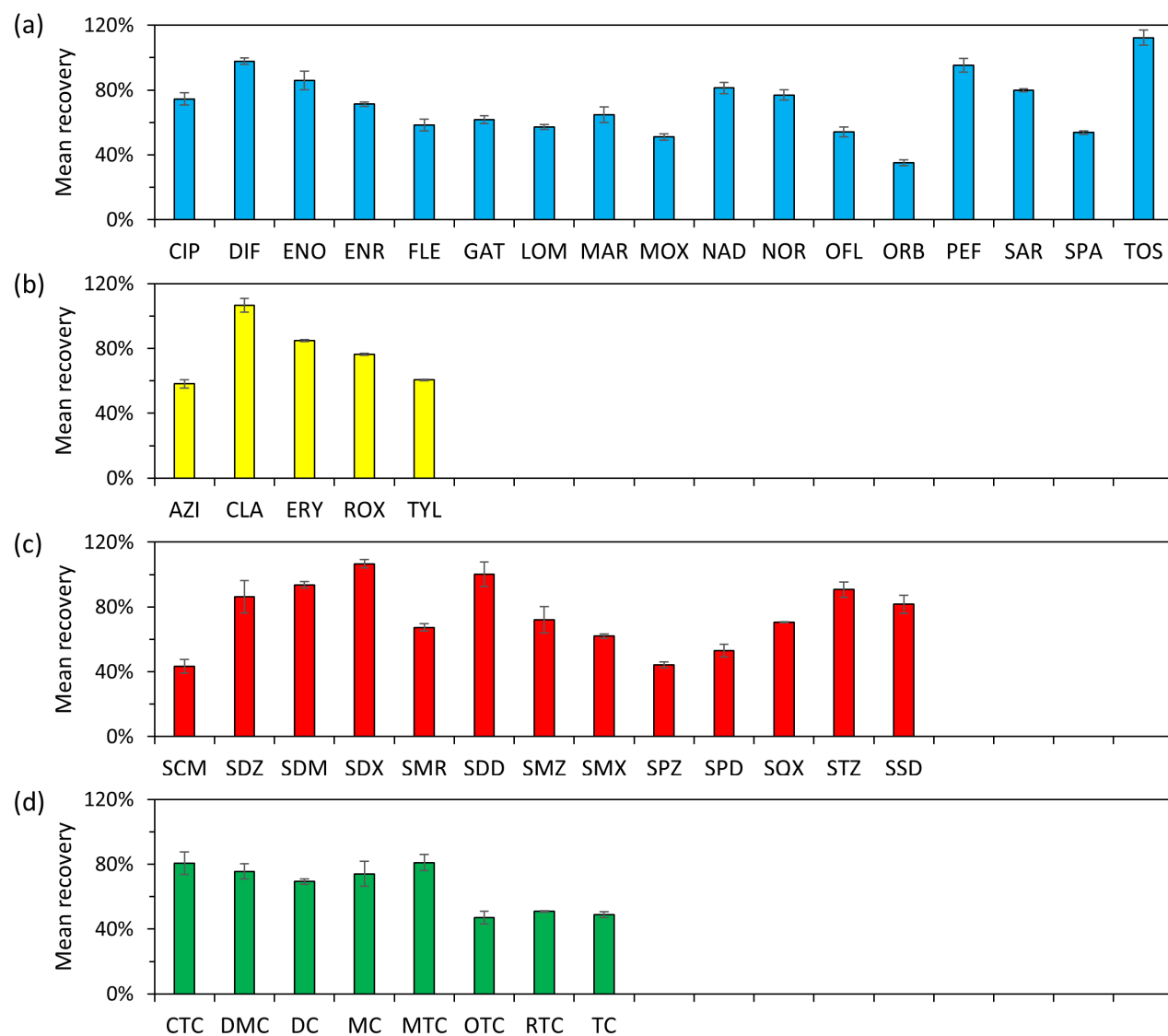
h: IS, internal standard used for quantitation of the listed CECs

i: Animal-labeled antibiotics

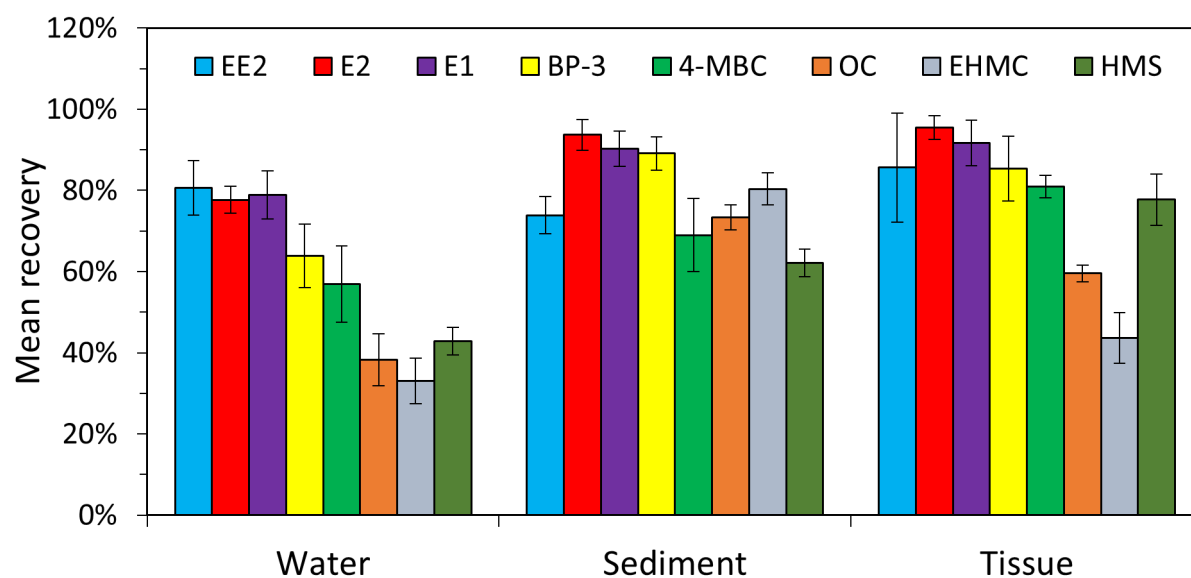


**Figure S1. Chromatograms of (a) 17 fluoroquinolone, (b) 5 macrolide, (c) 13 sulfonamide, and (d) 8 tetracycline standards at 10  $\mu\text{g/L}$  (approximately equivalent to 100  $\text{ng/L}$  concentrations following SPE). Note that complete LC separation was achieved for antibiotics with the same parent and/or fragment ions; acronyms are defined in Table S1.**





**Figure S2. Absolute recovery of the (a) 17 fluoroquinolone, (b) 5 macrolide, (c) 13 sulfonamide, and (d) 8 tetracycline analytes from water samples collected from HS-1 (as a representative site). Error bars are standard deviation ( $n = 3$ ) and chemical acronyms are defined in Table S1.**



**Figure S3. Absolute recovery of estrogenic hormones and UV-filters from water (100 mL), sediment (500 mg), and tissue (50 mg) samples collected from HS-1 (as a representative site). Error bars are standard deviation ( $n = 3$ ) and CEC acronyms are defined in Table S1.**

## REFERENCES

- (1) Jiménez-Lozano, E.; Marqués, I.; Barrón, D.; Beltrán, J.; Barbosa, J. Determination of pKa values of quinolones from mobility and spectroscopic data obtained by capillary electrophoresis and a diode array detector. *Analytica Chimica Acta* **2002**, *464* (1), 37–45.
- (2) Qiang, Z.; Adams, C. Potentiometric determination of acid dissociation constants (pKa) for human and veterinary antibiotics. *Water Research* **2004**, *38* (12), 2874–2890.
- (3) Tam, K. Y. Multiwavelength spectrophotometric resolution of the micro-equilibria of a triprotic amphoteric drug: Methacycline. *Mikrochimica Acta* **2001**, *136* (1–2), 91–97.
- (4) He, K.; Timm, A.; Blaney, L. Simultaneous determination of UV-filters and estrogens in aquatic invertebrates by modified quick, easy, cheap, effective, rugged, and safe extraction and liquid chromatography tandem mass spectrometry. *Journal of Chromatography A* **2017**, *1509*, 91–101.