

## Appendix A

Contaminants of emerging concern in a large temperate estuary.

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Table S1. List of all analytes measured in this study and their matrix reporting limits.

Table S2. Half-life, pKa,  $K_{ow}$ , usage, and mechanism of action for all detected analytes.

Table S3. Analytes that were not detected in effluent, estuary water, or fish tissue.

Table S4. Observed and predicted bioconcentration factors and sediment partition coefficients and observed concentrations for all analytes detected in water.

Table S5. Concentrations of detected analytes in both fish and water samples for all replicates.

Table S1. List of all analytes measured in this study and their matrix reporting limits.

	Class	Analyte class	Method water	Method tissue	Analyte	Abbrev	Common name	Water RL (ng/L)	Tiss RL (ng/g)
1	1	AP and APE	MLA 004	MLA 080	4-Nonylphenols	4-NP		9.1	0.46
2	1				4-Nonylphenol diethoxylates	NP2EO		14.8	0.46
3	1				4-Nonylphenol monoethoxylates	NP1EO		18.6	0.46
4	1				Octylphenol	4-OP		2.35	0.46
5	2	BPA (specific method)	MLA 082	MLA 084	Bisphenol A	BPA		1.92	1.01
6	3	HBCDD flame retardants		MLA 070	alpha-Hexabromocyclododecane	$\alpha$ -HBCDD			0.10
7	3				beta-Hexabromocyclododecane	$\beta$ -HBCDD			0.10
8	3				gamma-Hexabromocyclododecane	$\gamma$ -HBCDD			0.10
9	4	Hormones (negative)	MLA 072		17 alpha-Dihydroequilin			4.33	
10	4				17 alpha-Estradiol			4.33	
11	4				17 alpha-Ethinyl-Estradiol	EE2		6.05	
12	4				17 beta-Estradiol	E2		6.09	
13	4				Equilenin			0.87	
14	4				Equilin			10.6	
15	4				Estrone	E1		4.33	
16	5	Hormones (positive)	MLA 072		Allyl Trenbolone			1.02	
17	5				Androstenedione			2.16	
18	5				Androsterone			28.0	
19	5				Desogestrel			254	
20	5				Estriol			20.3	
21	5				Mestranol	MeEE2		54.1	
22	5				Norethindrone			4.33	
23	5				Norgestrel			4.33	
24	5				Progesterone			0.87	
25	5				Testosterone			1.04	

	Class	Analyte class	Method water	Method tissue	Analyte	Abbrev	Common name	Water RL (ng/L)	Tiss RL (ng/g)
26	6	Perfluorinated compounds	MLA 060	MLA 043	Perfluorobutanoate	PFBA		0.95	0.50
27	6				Perfluorobutanesulfonate	PFBS		1.90	1.01
28	6				Perfluorodecanoate	PFDA		0.95	0.50
29	6				Perfluorododecanoate	PFDoA		0.95	0.50
30	6				Perfluoroheptanoate	PFHpA		0.95	0.50
31	6				Perfluorohexanoate	PFHxA		0.95	0.50
32	6				Perfluorohexanesulfonate	PFHxS		1.90	1.01
33	6				Perfluorononanoate	PFNA		0.95	0.50
34	6				Perfluorooctanoate	PFOA		0.95	0.50
35	6				Perfluorooctanesulfonate	PFOS		1.90	1.01
36	6				Perfluorooctane sulfonamide	PFOSA		0.95	0.60
37	6				Perfluoropentanoate	PFPeA		0.95	0.50
38	6				Perfluoroundecanoate	PFUnA		0.95	0.50
39	7				Phthalate ester metabolites	MLA 059		Mono-methyl phthalate	MMP
40	7		Mono-n-butyl phthalate	MBP				0.20	
41	7		Mono-benzyl phthalate	MBzP				0.20	
42	7		Mono-cyclohexyl phthalate	MCHP				0.20	
43	7		Mono-3-carboxypropyl phthalate	MCPP				0.20	
44	7		Mono-(2-ethyl-5-hydroxyhexyl) phthalate	MEHHP				0.20	
45	7		Mono-2-ethylhexyl phthalate	MEHP				0.20	
46	7		Mono-(2-ethyl-5-oxohexyl) phthalate	MEOHP				0.20	
47	7		Mono-ethyl phthalate	MEP				0.20	
48	7		Mono-isononyl phthalate	MiNP				0.20	
49	8	PPCP (ANEG)	MLA 075	MLA 075	Bisphenol A	BPA		541	195
50	8				Furosemide		Lasix	43.3	15.6
51	8				Gemfibrozil		Lopid	1.62	0.58
52	8				Glipizide		Glucotrol	6.49	2.33
53	8				Glyburide (Glibenclamide)		Glynase	3.24	1.17

	Class	Analyte class	Method water	Method tissue	Analyte	Abbrev	Common name	Water RL (ng/L)	Tiss RL (ng/g)
54	8				Hydrochlorothiazide		Esidrix	16.0	5.76
55	8				Ibuprofen		Advil	16.2	5.84
56	8				2-Hydroxy-ibuprofen	Ibuprofen 2OH		86.5	31.1
57	8				Naproxen		Aleve	3.24	1.17
58	8				Triclocarban			3.24	1.17
59	8				Triclosan			64.9	23.3
60	8				Warfarin		Coumadin	1.62	1.55
61	9	PPCP (APOS)	MLA 075	MLA 075	Acetaminophen		Tylenol	16.2	5.84
62	9				Azithromycin		Zithromax	2.04	1.23
63	9				Caffeine			16.2	5.84
64	9				Carbadox			1.62	0.58
65	9				Carbamazepine		Tegretol	1.62	0.58
66	9				Cefotaxime		Claforan	6.49	2.33
67	9				Ciprofloxacin	Cipro	Cipro	6.49	5.58
68	9				Clarithromycin		Biaxin	1.62	0.58
69	9				Clinafloxacin			13.9	11.1
70	9				Cloxacillin			3.24	3.60
71	9				Dehydro Nifedipine			0.65	0.23
72	9				Digoxigenin			130	2.33
73	9				Digoxin		Lanoxin	6.49	2.81
74	9				Diltiazem		Cardizem	0.32	0.63
75	9				1,7-Dimethylxanthine (paraxanthine)		Theobromine	64.9	23.3
76	9				Diphenhydramine		Benadryl	0.65	0.23
77	9				Enrofloxacin		Baytril	3.24	1.17
78	9				Erythromycin-H2O		Ilotycin	2.49	0.90
79	9				Flumequine			1.62	1.41
80	9				Fluoxetine		Prozac	1.62	0.58
81	9				Lincomycin		Lincocin	3.24	1.36
82	9				Lomefloxacin		Maxaquin	3.53	1.50

	Class	Analyte class	Method water	Method tissue	Analyte	Abbrev	Common name	Water RL (ng/L)	Tiss RL (ng/g)
83	9				Miconazole		Monistat	1.62	1.14
84	9				Norfloxacin		Noroxin	18.4	18.6
85	9				Norgestimate			6.75	16.5
86	9				Ofloxacin		Ocuflox	1.62	0.58
87	9				Ormetoprim			0.65	0.23
88	9				Oxacillin		Bactocill	3.24	4.99
89	9				Oxolinic Acid			2.44	0.32
90	9				Penicillin G			3.24	1.20
91	9				Penicillin V			3.24	2.03
92	9				Roxithromycin			0.32	0.14
93	9				Sarafloxacin			16.2	5.84
94	9				Sulfachloropyridazine			1.62	0.67
95	9				Sulfadiazine			1.62	0.58
96	9				Sulfadimethoxine			0.32	0.18
97	9				Sulfamerazine			0.65	0.60
98	9				Sulfamethazine			1.34	0.89
99	9				Sulfamethizole			0.65	0.80
100	9				Sulfamethoxazole			0.75	0.68
101	9				Sulfanilamide			16.2	5.84
102	9				Sulfathiazole			1.62	0.96
103	9				Thiabendazole		Mintezol	1.62	0.58
104	9				Trimethoprim		Proloprim	1.62	0.58
105	9				Tylosin			6.49	2.33
106	9				Virginiamycin M1			3.68	3.23
107	10	PPCP (APOSX)	MLA 075	MLA 075	Alprazolam		Xanax	0.32	0.12
108	10				Amitriptyline		Elavil	0.37	0.12
110	10				10-hydroxy-amitriptyline	10-OH amitrip		0.16	0.06
109	10				Amlodipine		Norvasc	1.62	0.58
111	10				Benzoyllecgonine		Esterom	0.32	0.17
112	10				Benztropine		Cogentin	0.54	0.20

	Class	Analyte class	Method water	Method tissue	Analyte	Abbrev	Common name	Water RL (ng/L)	Tiss RL (ng/g)
113	10				Betamethasone		Luxiq	2.42	1.36
114	10				Cocaine			0.16	0.10
115	10				<i>N,N</i> -Diethyl- <i>meta</i> -toluamide	DEET	DEET	0.87	0.31
116	10				Desmethyldiltiazem			0.16	0.06
117	10				Diazepam		Valium	0.32	0.46
118	10				Fluocinonide		Lidex	6.49	5.94
119	10				Fluticasone propionate		Flonase	2.68	5.28
120	10				Meprobamate		Miltown	4.33	2.30
121	10				Methylprednisolone		Medrol	6.79	6.52
122	10				Metoprolol		Lopressor	3.01	1.81
123	10				Norfluoxetine		Seproxetine	1.62	0.58
124	10				Norverapamil			0.16	0.09
125	10				Paroxetine		Paxil	4.33	1.56
126	10				Prednisolone		Orapred	8.53	13.0
127	10				Prednisone		Deltasone	36.9	112
128	10				Promethazine		Phenergan	1.44	0.52
129	10				Propoxyphene		Darvon	0.32	0.12
130	10				Propranolol		Inderal	2.16	0.78
131	10				Sertraline		Zoloft	0.43	0.16
132	10				Simvastatin		Zocor	21.6	7.78
133	10				Theophylline		Elixophyllin	107	89.3
134	10				Trenbolone			4.33	1.56
135	10				Trenbolone acetate			0.38	0.25
136	10				Valsartan		Diovan	4.33	1.56
137	10				Verapamil		Calan	0.16	0.06
138	11	PPCP (BPOS)	MLA 075	MLA 075	Albuterol (salbutamol)		Proventil	3.05	0.28
139	11				Amphetamine			15.2	12.1
140	11				Atenolol		Tenormin	6.09	0.57
141	11				Atorvastatin		Lipitor	15.2	1.42
142	11				Cimetidine		Tagamet	6.09	0.57
143	11				Clonidine		Kapvay	15.2	1.42

Class	Analyte class	Method water	Method tissue	Analyte	Abbrev	Common name	Water RL (ng/L)	Tiss RL (ng/g)
144	11			Codeine			30.5	2.83
145	11			Cotinine			15.2	1.42
146	11			Enalapril		Vasotec	3.05	0.28
147	11			Hydrocodone			15.2	1.42
148	11			Metformin		Glucophage	30.5	2.83
149	11			Oxycodone		Oxycontin	6.09	0.69
150	11			Ranitidine		Rantacid	6.09	0.59
151	11			Triamterene		Dyrenium	3.05	0.28
152	12	Triclosan (specific method)	MLA 083	Triclosan			5.08	

RL is approximate reporting limit for each analyte in water or tissue. Method refers to the analytical method used for extraction and analytical determination for each compound by AXYS Analytical Services LTD, Sidney, B.C., Canada.



Table S2. Half-life, pKa, K<sub>ow</sub>, usage, and mechanism of action for all detected analytes.

	Analyte	Kow	pKa	Half-life			Use	MoA	WHO List
				Mammal	Fish	Sediment			
1	Albuterol	0.3	10.3	4 – 6 h (H)			Bronchodilation	β <sub>2</sub> -adrenergic receptor agonist	Y
2	Alprazolam	2.1	5.1/ 18.3	16 h (H)			Anti-anxiety	Unknown, CNS depressant	
3	Amitriptyline	5	9.4	10 – 50 h (H)			Antidepressant	SSRI	Y
4	10-OH-Amitrip	3.84	9.8/ 14.3				Antidepressant	SSRI	
5	Amlodipine	3.0	8.8	30 – 50 h			Hypertension	Calcium channel blocker	Y
6	Amphetamine	1.8	10.1	10 – 12 h (H)			Stimulant	↓ Uptake of adrenergics and dopamine, stimulates release of monoamines, and inhibits monoamine oxidase	
7	Androstenedione	2.7					Enhance testosterone	Precursor of male and female sex hormones	
8	Atenolol	0.2	9.6	7 h (H)			Antiarrhythmic	β <sub>1</sub> -selective adrenoceptor blocking agent	
9	Atorvastatin	5	4.46	20 h (H)			Lower cholesterol	↓ Hydroxymethylglutaryl-coenzyme A (HMG-CoA) reductase	
10	Azithromycin	4.0	8.74	68 h (H)	353 h (wb)	1 – 2.7 y <sup>2</sup>	Antibiotic	↓ Protein synthesis, binds 23S rRNA part of 50S ribosomal subunit	Y
11	Benzoyllecgonine	-0.3					Cocaine metabolite	Topical analgesic	
12	Benztropine	4.5		12 – 24 h (H)			Parkinson's disease	Muscarinic antagonist	
13	Bisphenol A	3.3	9.6	21 h (H)	139 h (wb)		Monomer of polycarbonate	Oxidative stress, endocrine disruption	
14	Caffeine	-0.1	14/0.7	5 h (H)	141 h <sup>1</sup>		Stimulant	CNS stimulant	

Analyte	Kow	pKa	Half-life			Use	MoA	WHO List
			Mammal	Fish	Sediment			
15 Carbamazepine	2.5	13.9	36 h (H)	71 hr <sup>1</sup>	495 d <sup>2</sup>	Anticonvulsant	Stabilizes inactivated state of voltage-gated sodium channels. Also GABA receptor agonist	Y
16 Cimetidine	0.4	6.8	3 h (H)			Inhibits gastric acid secretion	↓Histamine H2 receptor	
17 Ciprofloxacin	-1.1	6.1	3 – 7 h (H)	11 – 20 h (plasma)	6.3 y <sup>2</sup>	Antibiotic	↓DNA gyrase, a type II topoisomerase	Y
18 Clarithromycin	3.2	8.9	4 – 11 h (H)			Antibiotic	↓Protein synthesis, binds 23S rRNA part of 50S ribosomal subunit	Y
19 Cocaine	2.3	8.6	0.7 – 1.5 h (H)			Anesthetic and vasoconstrictor	↓ Dopamine uptake	
20 Codeine	1.1	10.6	3 h (H)			Analgesic	Opioid agonist	Y
21 Cotinine	-0.3		21 h (H)			Nicotine metabolite	Dopamine agonist via nicotinic receptors	
22 DEET	2		2.5 h (H)			Insect repellent	Binds odorant binding protein 1	
23 Dimethylxanthine 1,7	-0.2	9.9	6 – 10 h (H)			Primary metabolite caffeine	CNS stimulant	
24 Nifedipine (Dehydro)	2.8					Metabolite of Nifedipine (vasodilator)	Calcium channel blocker (class II)	Y
25 Diazepam	3	3.4	1.5 d (H)			Antianxiety, anticonvulsant, sedative	↑GABA activity	Y
26 Diltiazem	2.7	8.06	3 – 4.5 h (H)	117 h <sup>1</sup>		Vasodilator	Calcium channel blocker	
27 Desmethyldiltiazem	2.3–3.0	9.2–12.9				Hypertension, arrhythmia Metabolite of diltiazem	Calcium channel blocker	
28 Diphenhydramine	3.3	9.0	3 – 17 h (H)	34 h <sup>1</sup>	3 y <sup>2</sup>	Antihistamine	Inverse agonist of the histamine H1 receptor	

Analyte	Kow	pKa	Half-life			Use	MoA	WHO List
			Mammal	Fish	Sediment			
29 Enalapril	-0.1	3/5.4	<2h (H)			Reduce blood pressure	Angiotensin converting enzyme inhibitor	Y
30 Erythromycin-H2O	2.7	8.88	1.6 h (H)	216 h (wb)		Antibiotic	↓Protein synthesis, binds 23S rRNA part of 50S ribosomal subunit	Y
31 Estrone	3.1		19 h (H)			Naturally produced estrogen - hormone replacement	Binds estrogen receptor	
32 Fluocinonide	3.2					Glucocorticoid for eczema	Corticosteroid hormone receptor agonist	
33 Fluoxetine	4.1	9.8	4 – 5 d (H)		> 3 y <sup>2</sup>	Anti-depressant	SSRI	Y
34 Furosemide	2	3.8/7.5	1.5 h (H)			Diuretic	Inhibits Na-K-Cl cotransporter	Y
35 Gemfibrozil	4.77	4.5	1.5 h (H)	19 h (plasma)	227 d <sup>2</sup>	↓Lipids	PPAR α agonist	
36 Glipizide	1.9	5.9	2 – 5 h (H)			Hypoglycemic agent for type 2 diabetes	Binds to ATP-sensitive K-channel receptors	
37 Glyburide	4.8		1.5 h (H)			Antidiabetic	Regulator of ATP-sensitive K+ channels and insulin release	Y
38 γ-HBCDD	7.1					Flame retardant	↑FSH and protein kinase B	
39 α-HBCDD	5.6 – 7.7	-	Months in fat			Flame retardant	↑FSH and protein kinase B	
40 Hydrochlorothiazide	-0.1	7.9				Diuretic	Inhibits NaCl symporters	Y
41 Hydrocodone	2.2	8.23	3.8 h (H)			Narcotic analgesic	Opioid agonist	
42 Ibuprofen	3.5	4.9	2 h (H)	32 h <sup>1</sup>		Nonsteroidal anti-inflammatory	↓Cyclooxygenase	Y
43 2-OH-Ibuprofen	2.1					Ibuprofen metabolite	-	
44 Lincomycin	0.2	7.6	4 – 6 h (H)			Antibiotic	↓Protein synthesis, binds 23S rRNA part of 50S ribosomal subunit	

Analyte	Kow	pKa	Half-life			Use	MoA	WHO List
			Mammal	Fish	Sediment			
45 MBP	3.1					Metabolite of DBP plasticizers	Endocrine / metabolic disruptor	
46 MEHP	4					Metabolite of DEHP plasticizers	Endocrine / metabolic disruptor	
47 Meprobamate	0.7		6 – 16 h (H)			Carbamate for anxiety	Adrenergic beta-antagonist	
48 Metformin	-1.3	12.4	8 – 12 h (H)			Hypoglycemic agent	↑AMP-activated protein kinase	Y
49 Metoprolol	1.9	9.68	3 – 7 h (H)			Arrhythmia, hypertension	Adrenergic beta-1 antagonist	Y
50 Miconazole	5.9 – 6.1	6.8	24 h		3.8 y <sup>2</sup>	Antifungal	↓Synthesis of ergosterol	Y
51 Naproxen	3.3	4.15	13 h (H)			Analgesic and antipyretic	↓Cyclooxygenase	
52 Norfluoxetine	3.5	9.8	4 – 16 d (H)			Metabolite of fluoxetine	SSRI	
53 Norverapamil	3.3	10.3	5 h			Metabolite of verapamil	Calcium channel blocker	
54 4-NP	5.76	10	3 h (H)	20 h	14 – 99 d <sup>4</sup>	Emulsifiers, solubilizers	Oxidative stress, endocrine disruption	
55 NP1EO	5.8				69 – 116 d <sup>4</sup>	Nonionic surfactant	Potential endocrine disruptor	
56 NP2EO	5.6				16 d (12.7 °C) <sup>3</sup>	Nonionic surfactant	Potential endocrine disruptor	
57 Ofloxacin	-0.4	5.97/9.28	16 h (H)		3.8 y <sup>2</sup>	Antibacterial	↓DNA gyrase	
58 Ormetoprim	1.2			15 – 400 h (organs); 45 – 99 d (fat & skin)		Antiprotozoal	Folic acid antagonist	

Analyte	Kow	pKa	Half-life			Use	MoA	WHO List
			Mammal	Fish	Sediment			
59 Oxycodone	1.2	8.3	0.4 h (H)			Analgesic	Opioid agonist	
60 Paroxetine	3.5		21 h (H)			Treat depression	SSRI	
61 PFBA	2.2					Breakdown product of PFCs		
62 PFBS	2.3		30 d (H)			Replaces PFOS		
63 PFDA	6.3					Surfactant	↑ Peroxisomal beta-oxidation	
64 PFHpA	4.3					Surfactant		
65 PFHxA	3.6					Breakdown product of PFCs		
66 PFHxS	3.7		Years (H)					
67 PFNA	5.6					Breakdown product of PFCs	↑ Peroxisomal beta-oxidation, apoptosis	
68 PFOA	4.9	2.8	4.4 y (H)			Surfactant	↑ Peroxisomal enzymes	
69 PFOS	6.3	0.14	5.4 y (H)			Surfactant	Oxidative stress, lipid peroxidation, apoptosis	
70 PFOSA	4.8		8.7 y (H)			Surfactant, Metabolized to PFOS	Neurotoxic, uncouple oxidative phosphorylation	
71 PFPeA	2.9					Breakdown product of PFCs		
72 Promethazine	4.8	9.1	9 – 16 (H)			Antihistamine, antiemetic, anticholinergic	Histamine H1-blocking, antimuscarinic	
73 Propoxyphene	4.2		6 – 12 h (H)			Narcotic analgesic	Opioid agonist	
74 Propranolol	3	9.42	4 h (H)			Arrhythmia, angina, hypertension	Beta-adrenergic antagonist	Y
75 Ranitidine	0.3		2 – 3 h (H)			Treat ulcers	Histamine H2 receptor antagonist	Y

Analyte	Kow	pKa	Half-life			Use	MoA	WHO List	
			Mammal	Fish	Sediment				
76	Roxithromycin	3.1		12 h (H)		Antibiotic	↓Protein synthesis, binds 23S rRNA part of 50S ribosomal subunit		
77	Sertraline	5.1	9.5	25-26 h		Anti-depressant	SSRI		
78	Simvastatin	4.7		3 h (H)		Reduce lipids	↓HMG-CoA reductase	Y	
79	Sulfadiazine	-0.1	6.36		26 – 96 h (plasma)	Antibiotic	↓Folate production	Y	
80	Sulfadimethoxine	1.6			99 h (wb)	Antibiotic	↓Folate production		
81	Sulfamerazine	0.1				Antibiotic	Binds to dihydrofolate synthetase, ↓folate		
82	Sulfamethoxazole	0.9	1.6/5.7	10 h (H)	26 h (wb)	Antibiotic	Cytochrome P450 2C9 Inhibitor, ↓folate	Y	
83	Testosterone	3.3		2 h (H)	2 h (wb)	403 (soil)	Androgenic steroid	Control pituitary LH and FSH secretion	Y
84	Thiabendazole	2.5	4.6	1.7 h (H)		403 d	Nematicide, fungicide	↓Fumarate reductase	
85	Triamterene	1		4.2 h (H)			Diuretic	↓Na reabsorption via Na channels	
86	Triclocarban	5.3	12.7	10 h (H)	1 h (wb)	> 3 y <sup>2</sup>	Antiseptic	↓Fatty acid synthesis	
87	Triclosan	4.76	7.9	21 h (H)		187 d	Antiseptic	↓Fatty acid synthesis	
88	Trimethoprim	0.9	7.1	11 h (H)	50 – 100 h (wb)		Antibiotic	↓Dihydrofolate reductase	Y
89	Valsartan	4.4	3.8	6 h (H)			Cardiac conditions	Angiotensin II receptor antagonist	
90	Verapamil	3.8	8.9	3 h			Hypertension, angina, arrhythmia	Calcium channel (L-type) blocker	Y
91	Virginiamycin M1	2.5					Antibiotic	↓Peptide chain (peptidyl-tRNA) linked to 50S ribosome and aminoacyl-tRNA	
92	Warfarin	2.7	5.1	40 h (H)			Anitcoagulant	↓Synthesis vitamin K-dependent coagulation factors	Y

All values for Kow, pKa, human half-life, usage, and mechanism or mode of action (MoA) from PubChem (2015), Toxnet (2015), EWG (2015), DrugBank (2015), Chemspider (2015), and Wikipedia (2015). List of essential medicines from WHO (2015). Fish half-life from Phish-Pharm or literature. Human half-life mostly for plasma. If compound exhibits acid and base ionization, the pKa for acid is shown first, then pKa for base. pKa1 is followed by pKa2. ↓↑Decrease or increase for parameter. Abbreviations are: H= *Homo sapiens*. h= hours, d= days, y= years, wb= whole body. PFC is perfluorinated compounds. SSRI is selective serotonin reuptake inhibitor. PPAR $\alpha$  is peroxisome proliferator activator receptor alpha, FSH = Follicle-stimulating hormone, HMG-CoA is 3-hydroxy-3-methylglutaryl coenzyme A. Analyte abbreviations in Table S1. DBP is dibutyl phthalate, and DEHP is diethylhexyl phthalate. References: 1. Wang and Gardinali (2012). 2. Walters et al. (2010), 3. Gonzalez et al. (2012), 4. Yuan et al. (2004).

Table S3. Analytes that were not detected in effluent, estuary water, or fish tissue.

	Class	Analyte class	Analyte	RL	
				Water ng/L	Tissue ng/g
1	1	AP and APE	Octylphenol	2.35	0.46
2	3	HBCDD flame retardants	beta-HBCDD		0.10
3	4	Hormones (negative)	17 alpha-Dihydroequilin	4.33	
4	4		17 alpha-Estradiol	4.33	
5	4		17 alpha-Ethinyl-Estradiol	6.05	
6	4		17 beta-Estradiol	6.09	
7	4		Equilenin	0.87	
8	4		Equilin	10.6	
9	5	Hormones (positive)	Allyl Trenbolone	1.02	
10	5		Androsterone	28.0	
11	5		Desogestrel	254.0	
12	5		Estriol	20.3	
13	5		Mestranol*	168	
14	5		Norethindrone	4.33	
15	5		Norgestrel	4.33	
16	5		Progesterone	0.87	
17	6	Perfluorinated	PFUnA	0.95	0.50
18	6		PFDoA	0.95	0.50
19	7	Phthalate ester metabolites	MMP	0.20	
20	7		MEP	0.20	
21	7		MBzP	0.20	
22	7		MEOHP	0.20	
23	7		MEHHP	0.20	
24	7		MCPP	0.20	
25	7		MCHP	0.20	
26	7		MiNP	0.20	
27	9	PPCP (APOS)	Acetaminophen	16.2	5.84
28	9		Carbadox	1.62	0.58
29	9		Cefotaxime	6.49	2.33
30	9		Clinafloxacin	13.9	11.1
31	9		Cloxacillin	3.24	3.60



Class	Analyte class	Analyte	RL	
			Water ng/L	Tissue ng/g
32	9	Digoxin	6.49	2.81
33	9	Digoxigenin	130	2.33
34	9	Enrofloxacin	3.24	1.17
35	9	Flumequine	1.62	1.41
36	9	Lomefloxacin	3.53	1.50
37	9	Norfloxacin	18.4	18.6
38	9	Norgestimate	6.75	16.5
39	9	Oxacillin	3.24	4.99
40	9	Oxolinic Acid	2.44	0.32
41	9	Penicillin G	3.24	1.2
42	9	Penicillin V	3.24	2.03
43	9	Sarafloxacin	16.2	5.84
44	9	Sulfachloropyridazine	1.62	0.67
45	9	Sulfamethazine	1.34	0.89
46	9	Sulfamethizole	0.65	0.80
47	9	Sulfanilamide	16.2	5.84
48	9	Sulfathiazole	1.62	0.96
49	9	Tylosin	6.49	2.33
50	10	PPCP (APOSX) Betamethasone	2.42	1.36
51	10	Fluticasone propionate	2.68	5.28
52	10	Methylprednisolone	6.79	6.52
53	10	Prednisolone	8.53	13.0
54	10	Prednisone	36.9	112
55	10	Theophylline	107	89.3
56	10	Trenbolone	4.33	1.56
57	10	Trenbolone acetate	0.38	0.25
58	11	PPCP (BPOS) Clonidine	15.2	1.42

RL = reporting limit. Abbreviations in Table S1. \* Mestranol was reported as detected in effluent (439 and 457 ng/L) and estuarine water (113 and 175 ng/L) but flagged (K-flag). A peak was detected but it did not meet quantification criteria. An interference at the expected mestranol retention time precluded positive identification for this compound.

Table S4. Observed concentrations for all analytes detected in water, bioconcentration factors, and sediment-water partition coefficients.

Analytes	<u>Sinclair Inlet</u>		<u>Puyallup</u>		<u>Nisqually</u>	<u>Partitioning</u>	
	Effluent	Estuary	Effluent	Estuary	Estuary	BCF	Log Koc
	2014 ng/L	2014 ng/L	2014 ng/L	2013 ng/L	2013 ng/L		
1 Albuterol	41	12	36			3	1.4
2 Alprazolam	3.0		4.0				
3 Amitriptyline	119		88			1,226	4.05
4 Amitriptyline 10-OH	60	0.19	43	0.21			
5 Amlodipine	9.7		26			4.4	2.3
6 Amphetamine	164	29	67	2.2			
7 Androstenedione	8.4					26	2.9
8 Atenolol	1700	22	2440	3.4	1.2		
9 Atorvastatin			68			56	
10 Azithromycin	629	2.2	261			200	3.49
11 Benzoylcegonine	293	0.51	151	0.78	0.5		
12 Benzotropine	0.93		0.57			400	5.0
13 Bisphenol A	350	2.8	4290	4.3		5 – 73*	2.1 – 3.59*
14 Caffeine	1170		152			2 <sup>1</sup>	
15 Carbamazepine	510		735	1.9		1.4 <sup>1</sup> , 4.2 (plasma) <sup>8</sup>	
16 Cimetidine			194			1.2	1.6
17 Ciprofloxacin	192		158		7.3	3	4.78*
18 Clarithromycin	52		181			56	2.17
19 Cocaine	59		8.5		0.28	3	2.78
20 Codeine	178		290				
21 Cotinine	340		115			3	2.01
22 DEET	684	2.4	23	5.3	8.4	2*	2.48
23 Diazepam	2.2		1.5			33	2.8*
24 Diltiazem	390	0.75	425	0.52		16 <sup>1</sup> 24 (plasma) <sup>8</sup>	
25 Desmethyldiltiazem	148		82				
26 Dimethylxanthine-1,7	2060		873				
27 Diphenhydramine	1240	1.5	1030	1.2	0.96	16 <sup>1</sup>	2.58
28 Enalapril			5.6				
29 Erythromycin-H2O	138		87	3.3		49	2.75

Analytes	<u>Sinclair Inlet</u>		<u>Puyallup</u>		<u>Nisqually</u>	<u>Partitioning</u>	
	Effluent	Estuary	Effluent	Estuary	Estuary	BCF	Log Koc
	2014 ng/L	2014 ng/L	2014 ng/L	2013 ng/L	2013 ng/L		
30 Estrone	58		4.5			54	2.7 – 4.3*
31 Fluoxetine	57		60			30 (pH 8) <sup>2</sup>	
32 Furosemide	1290		994			3	2.48
33 Gemfibrozil	1640	3.4	1360	4.5		3, 63 (plasma) <sup>3</sup>	2.63
34 Glipizide	22		22				
35 Glyburide	11		7.6				
36 Hydrochlorothiazide	578		411				
37 Hydrocodone	74		69			9	3.38
38 Ibuprofen	1060		116			28 <sup>1</sup> , 18,667 (plasma) <sup>3</sup>	3.5
39 Ibuprofen 2-OH	4550		1160			28	
40 Lincomycin			27			3	1.8
41 MBP				289	491		
42 MEHP			0.41				
43 Meproamate	623		513			3	1.8
44 Metformin	29300	832	82700	105			
45 Metoprolol	805		835			1.3	1.8
46 Miconazole			4.9				
47 Naproxen	701		106			3, 28 (plasma) <sup>8</sup>	2.5
48 Nifedipine (dehydro)	15		13			33	
49 NP2EO	2610		1690				
50 NP1EO	1760		1220				
51 NP (4-)	506		1690	41	14	945 <sup>4</sup>	4.5
52 Norfluoxetine	28		17			130 (pH 8) <sup>2</sup>	
53 Norverapamil	13		14				
54 Ofloxacin	387		108			3	4.64*
55 Oxycodone	158		231			3	2.08
56 Paroxetine	42		6.6				
57 PFBA			6.7				
58 PFBS	13						
59 PFHpA	7.5		3.0				
60 PFHxA	53		15			4,750 <sup>5</sup>	

Analytes	<u>Sinclair Inlet</u>		<u>Puyallup</u>		<u>Nisqually</u>	Partitioning	
	Effluent	Estuary	Effluent	Estuary	Estuary	BCF	Log Koc
	2014 ng/L	2014 ng/L	2014 ng/L	2013 ng/L	2013 ng/L		
61 PFHxS	55						
62 PFNA			2				
63 PFOA	12		7.6			7.3 <sup>5</sup>	2.96 <sup>6</sup>
64 PFOS	461					1,010 <sup>5</sup>	3.79 <sup>6</sup>
65 PFPeA	4.7		3.4				
66 Promethazine			3.8				
67 Propoxyphene	1.9		0.70			260	4.9
68 Propranolol	76		109				
69 Ranitidine			494		0.75		
70 Roxithromycin			3.8				
71 Sertraline	116		89			138 (plasma) <sup>8</sup>	
72 Simvastatin			34			800	3.92
73 Sulfadimethoxine		0.46	8.2				
74 Sulfamethoxazole		4.1	1380	3.4	1.5	3	1.86
75 Testosterone		1.9				72	3.34
76 Thiabendazole	27		24			20	3.56
77 Triamterene	151		156				
78 Triclocarban	12		17			80 <sup>*</sup>	4.08 <sup>*</sup>
79 Triclosan	538	5.2	250			90 <sup>*</sup> , 4157 <sup>7</sup>	3.54 <sup>*</sup>
80 Trimethoprim	742		852	2.3		3	1.87
81 Valsartan	2010		3000	5.4		3	4.36
82 Verapamil	41		44			175 (plasma) <sup>8</sup>	
83 Warfarin			6.2			28	1.5 – 2.96
N detected	66	16	77	17	10		

Concentrations are quantified values from each waste water treatment plant (WWTP) effluent and water from the receiving estuary. All blank values indicate <RL (see Table S1). Bioconcentration factors (BCF) and organic carbon normalized sediment-water partition coefficients (Koc) are estimated values from the literature, unless noted. BCF for whole-body unless noted. Koc shown as log<sub>10</sub> values. All estimated BCF and Koc values from PubChem (2015). \* indicates observed values listed in PubChem (2015). See Table S1 for all analyte abbreviations. References. 1. Wang and Gardinali (2013), 2. Nakamura et al. (2008), 3. Brown et al. (2007), 4. USEPA (2005), 5. Inoue et al. (2012), 6. Arvaniti et al. (2014), 7. Orvos et al. (2002), 8. Fick et al. (2010).



Analytes	Sinclair Inlet					Puyallup						Nisqually				Hatch
	Eff	Est	salmon		sculp	Eff	Est	salmon		sculp		Est	salmon	sculp		salmon
			A	B				A	B	A	B			A	B	
	2014	2014	2014	2014	2014	2014	2013	2014	2014	2014	2013	2013	2014	2014	2013	2014
ng/L	ng/L	ng/g	ng/g	ng/g	ng/L	ng/L	ng/g	ng/g	ng/g	ng/g	ng/L	ng/g	ng/g	ng/g	ng/g	ng/g
Miconazole					4.9		1.4	1.8								
Norfluoxetine	28				17		3.2	2.7				0.68				
Norverapamil	13		0.20		0.20	14		0.47	0.39			0.12	0.25			
4-NP	506		30	33	27	1690	41	76	33	35	35	14	76	29	7.7	51
NP1EO	1760		3.0	2.2	3.0	1220		57	60	4.9			1.3	2.2		1.3
NP2EO	2610		1.4	2.2	1.9	1690		49	51	17	6.2		2.1	7.5		3.1
Ormetoprim				44				1010	1600				642			
PFDA			0.78													
PFOS	461		34	1.4	1.4						1.1		1.2			
PFOSA					0.82						2.2					
Ranitidine					0.97	494		0.82				0.75	1.1			
Sertraline	116					89		17	4.9	0.21						
Sulfadiazine			0.88													
Sulfadimethoxine		0.46		0.34		8.2		16.2	9.8				17			
Sulfamerazine									0.51							
Triclocarban	12					17		4.0	6.5							
Triclosan	411	5.2				183		26	23							
Verapamil	41		0.30		0.25	44		0.60	0.54		0.07		0.12	0.27		
Virginiamycin					8.0			10			34					
N detected for sample			13	12	15			26	24	9	9		13	7	5	7
N detected for matrix and site			19					28		15				9		

Fish and effluent (Eff) sampled in 2013 and 2014. Estuary water (Est) sampled in 2013. Hatch = Voight's Creek Hatchery (Puyallup watershed) sampled on 29 May 2014. Salmon is Chinook salmon (*Oncorhynchus tshawytscha*) and Sculp = staghorn sculpin (*Leptocottus armatus*). See Table S1 for abbreviations and reporting limits.

## Citations

- Arvaniti O.S., Andersen H.R., Thomaidis N.S., Stasinakis A.S. 2014. Sorption of perfluorinated compounds onto different types of sewage sludge and assessment of its importance during wastewater treatment. *Chemosphere* 111:405-411.
- Brown J.N., Paxeus N., Forlin L., Larsson D.G.J. 2007. Variations in bioconcentration of human pharmaceuticals from sewage effluents into fish blood plasma. *Environ Toxicol Pharm* 24:267-274.
- Chemspider. 2015. <http://www.chemspider.com> (last accessed 30 July 2015)
- Drugbank. 2015. <http://www.drugbank.ca/> (last accessed 30 July 2015)
- EWG. 2015. <http://www.ewg.org/sites/humantoxome/> (last accessed 30 July 2015)
- Fick J., Lindberg R.H., Parkkonen J., Arvidsson B., Tysklind M., Larsson D.G.J. 2010. Therapeutic levels of levonorgestrel detected in blood plasma of fish: results of screening rainbow trout exposed to sewage effluents. *Environ Sci Tech* 44:2661-2666.
- Gonzalez M.M., Camacho-Munoz, Santos JL, Aparicio I, and Alonso E. 2012. Degradation and environmental risk of surfactants after the application of compost sludge to the soil. *Waste Management* 32:1324-1331.
- Inoue Y., Hashizume N., Yakata N., Murakami H., Suzuki Y., Kikushima E., Otsuka M. 2012. Unique physiochemical properties of perfluorinated compounds and their bioconcentration in common carp *Cyprinus carpio* L. *Arch Environ Contam Toxicol* 62:672-680.
- Nakamura Y., Yamamoto H., Sekizawa J., Kondo T., Hirai N., Tatarazako N. 2008. The effects of pH on fluoxetine in Japanese medaka (*Oryzias latipes*): acute toxicity in fish larvae and bioaccumulation in juvenile fish. *Chemosphere* 70:865-873.

- Orvos D.R., Versteeg D.J., Inauen J., Capdevielle M., Rothenstein A.,  
Cunningham V. 2002. Aquatic toxicity of triclosan. *Environ Toxicol Chem*  
21:1338-1349.
- U.S. FDA. 2014. PhishPharm database. [Accessed 30 July 2015].  
<http://www.fda.gov/AnimalVeterinary/ScienceResearch/ToolsResources/Phish-Pharm/> (last accessed 30 July 2015)
- Pubchem. 2015. National Center for Biotechnology Information. PubChem  
Compound Database; <https://pubchem.ncbi.nlm.nih.gov> (last accessed 30  
July 2015)
- Toxnet. 2015. <http://toxnet.nlm.nih.gov/> (last accessed 30 July 2015)
- USEPA. 2005. Aquatic Life Ambient Water Quality – Nonylphenol. EPA-822-R-05-  
005 Office of Water. Washington, DC
- Walters E., McClellan K., Halden R.U. 2010. Occurrence and loss over three  
years of 72 pharmaceuticals and personal care products from biosolid-soil  
mixtures in outdoor mesocosms. *Water Res* 44:6011-6020.
- Wang J., Gardinali P.R. 2012. Analysis of selected pharmaceuticals in fish and  
the freshwater bodies directly affected by reclaimed water using liquid  
chromatography-tandem mass spectrometry. *Anal Bioanal Chem* 404:2711-  
2720.
- Wikipedia. 2015. <https://www.wikipedia.org/> (last accessed 30 July 2015)
- WHO. 2015. World Health Organization Model List of Essential Medicines. 19th  
List. <http://www.who.int/medicines/publications/essentialmedicines/en/> (last  
accessed 30 July 2015)
- Yuan S.Y., Yu C.H., Chang B.V. 2004. Biodegradation of nonylphenol in river  
sediment. *Environ Poll* 127:425-430.