Table 1. Physical properties and chemicals analyzed for in water or bottom sediment samples.

[MRL, minimum reporting level; EDP, endocrine-disrupting potential; K_{ow}, octanol-water partition coefficient; CASRN, Chemical Abstracts Services Registry Number; µS/cm, microsiemens per centimeter at 25 degrees Celsius (°C); FIELD, field sample; mg/L, milligrams per liter; --, not available; NWQL, National Water Quality Laboratory; USGS–NRP, U.S. Geological Survey National Research Program (laboratory); EDTA, ethylenediaminetetraacetic acid; NTA; nitrilotriacetic acid; NPEC, nonlyphenol ethoxycarboxylate; µg/L, micrograms per liter; ng/L, nanograms per liter;; S, suspected; K, known; E or e, remark code estimated concentration reported; F, fungicide; H, herbicide; I, insecticide; GUP, general-use pesticide; FR, flame retardant; WW, wastewater; manuf., manufacturing; %, percent; >, greater than; CP, combustion product; PAH, polycyclic aromatic hydrocarbon; UV, ultraviolet; NA, not applicable; Compounds measured in both water and sediment samples unless otherwise marked].

Property/chemical name	MRL[1]	Log K_{ow}[3]	CASRN[4]	Possible compound uses or sources[5]
Nutrients Analyzed in Water at the USGS National Water Quality Laboratory (mg/L)				
Ammonia plus organic nitrogen, filtered	0.1	--	17778-88-0	Nutrient
Ammonia plus organic nitrogen, unfiltered	0.1	--	17778-88-0	Nutrient
Ammonia as nitrogen	0.02	--	7664–41–7	Nutrient
Nitrite plus nitrate	0.04	--	--	Nutrient
Nitrogen, nitrite	0.002	--	14797–65–0	Nutrient
Orthophosphate	0.008	--	14265–44–2	Nutrient
Total phosphorus, filtered	0.006	--	7723–14–0	Nutrient
Total phosphorus, unfiltered	0.008	--	7723-14-0	Nutrient
Chemicals Analyzed in Water at Larry Barber's USGS National Research Program Laboratory(ng/L)				
4-Nonylphenol[1]	100	5.92	25154–52–3	Surfactant metabolite.
4-Nonylphenolmonoethoxylate[1]	50	5.58	27986–36–3	Surfactant metabolite.
4-Nonylphenoldiethoxylate[1]	50	--	9016–45–9	Surfactant metabolite.
4-*tert*-Octylphenol[1]	5	5.28	140–66–9	Surfactant metabolite.
4-*tert*-Octylphenolmonoethoxylate[1]	5	--	9036–19–5	Surfactant metabolite.
4-*tert*-Octylphenoldiethoxylate[1]	5	--	2315–64–0?	Surfactant metabolite.
Bisphenol A[1]	5	3.64	80–05–7	FR, manuf. polycarbonate resins, antioxidant.
Fluoxetine[1]	50	--	58–08–2	Stimulant.
Fluvoxamine[1]	5	--	57–88–5	Animal steroid
Diethylpthalate[1]	5	--	--	Pharmaceutical
Triclocarban[1]	50	--	134–62–3	I, urban uses, mosquito repellent.
Triclosan[1]	5	--	3380–34–5	Antimicrobial.
17β-estradiol[1]	5	--	--	Reproductive Hormone
17α-ethynylestradiol[1]	5	--	--	Ovulation inhibitor
Estrone[1]	5	--	--	Reproductive hormone
Estriol[1]	5	--	--	Reproductive hormone
1,4-Dichlorobenzene[1]	5	3.28	106–46–7	Moth repellent, fumigant, deodorant.
2,6-Di-*tert*-butyl-1,4-benzoquinone[1]	5	4.07	719–22–2	Antioxidant by-product.

5-methyl-1H-benzotriazole[1]	5	1.71	136–85–6	Antioxidant in antifreeze and deicers
N,N,diethyl-*meta*-toluamide[1]	5	2.26	134–62–3	I, urban uses, mosquito repellent.
4-Androstene-3,17-dione [1]	5	--	--	Anabolic agent and natural steroid
Testosterone [1]	5	--	--	Reproductive hormone
D6-Bisphenol A (percent)	--	--	86588–58–1	Surrogate standard.
D21-2,6-Di-*tert*-butyl-4-methylphenol (percent)	--	--	64502–99–4	Surrogate standard.
4-*n*-Nonylphenol (percent)	--	--	104–40–5	Surrogate standard.
4-*n*-Nonylphenolmonoethoxylate (percent)	--	--	--	Surrogate standard.
4-*n*-Nonylphenoldiethoxylate (percent)	--	--	--	Surrogate standard.
D4-17-*β*-Estradiol (percent)	--	--	66789–03–5	Surrogate standard.
D7-Cholesterol (percent)	--	--	--	Surrogate standard.
Pharmaceuticals Analyzed in Water at the USGS National Water Quality Laboratory(ug/L)				
1,7-Dimethylxanthine[1]	0.12	-0.39	611-59-6	Precursor is a stimulant
Acetaminophen[1]	0.08	0.27	103-90-2	Analgesic
Albuterol	0.06	0.64	18559-94-9	Bronchodilator
Caffeine[1]	0.20	.16	58–08–2	Beverages, diuretic, very mobile/biodegradable
Carbamazepine[1]	0.04	2.25	298-46-4	Antiepileptic
Codeine[1]	0.04	1.28	76-57-3	Opiate agonist
Cotinine[1]	0.026	.34	486–56–6	Primary nicotine metabolite
Dehydronifedipine[1]	0.08	--	67035-22-7	Precursor is an antiangial
Diltiazem[1]	0.08	2.79	42399-41-7	Antihypertensive
Diphendydramine[1]	0.04	3.11	58-73-1	Antipruritic
Fluoxetine[1]	--		54739-18-3	SSRI Antidepressant
Sulfamethoxazole[1]	0.16	0.48	723-46-6	Antibiotic
Thiabendazole[1]	0.06	2.00	148-79-8	Anthelmintic, fungacide
Trimethoprim[1]	0.02	0.73	738-70-5	Antibiotic
Warfarin[1]	0.1	2.23	81-81-2	Anticoagulant, rodenticide
Carbamazepine-d10 (percent)	--	--		Surrogate standard
Ethyl Nicotinate-d4 (percent)	--	--		Surrogate Standard
Chemicals analyzed in Bottom Sediment at the USGS National Water Quality Laboratory (ng/g)				
1,4-Dichlorobenzene[1]	50	3.28	106–46–7	Moth repellent, fumigant, deodorant
1-Methylnaphthalene[1]	50	3.72	90–12–0	2–5% of gasoline, diesel fuel, or crude oil
2,6-Dimethylnaphthalene[1]	50	4.26	581–42–0	Percent in diesel/kerosene (trace in gasoline)
2-Methylnaphthalene[1]	50	3.72	91–57–6	2–5% of gasoline, diesel fuel, or crude oil
3-*beta*-Coprostanol[1]	500	8.82	360–68–9	Carnivore fecal indicator.
3-Methyl-1H-indole (skatol) [1]	50	2.60	83–34–1	Fragrance, stench in feces, and coal tar
3-*tert*-Butyl-4-hydroxyanisole[1]	150	3.50	25013–16–5	Antioxidant

4-Cumylphenol[1]	50	4.12	599–64–4	Surfactant metabolite
4-*n*-Octylphenol[1]	50	5.50	1806–26–4	Surfactant metabolite
4-Nonylphenol[1]	750	5.92	84852–15–3	Surfactant metabolite
4-Nonylphenoldiethoxylate[1]	1000	--	--	Surfactant metabolite
4-Nonylphenolmonoethoxylate[1]	500	5.58	--	Surfactant metabolite
4-*tert*-Octylphenol[1]	50	5.28	140–66–9	Surfactant metabolite
4-tert-Octylphenoldiethoxylate[1]	50	--	--	Surfactant metabolite
4-tert-Octylphenolmonoethoxylate[1]	250	--	--	Surfactant metabolite
Acetophenone [1]	150	1.67	98–86–2	Fragrance and flavor
Acetyl-hexamethyl-tetrahydronaphthalene (tonalide) [1]	50	6.35	21145–77–7	Musk fragrance
Anthracene [1]	50	4.35	120–12–7	CP, component of tar, diesel, or crude oil
Anthraquinone[1]	50	3.34	84–65–1	Manuf. dye/textiles, seed treatment, bird repellent
Atrazine[1]	100	2.82	1912–24–9	Selective triazine herbicide
Benzo[a]pyrene [1]	50	6.11	50–32–8	CP, regulated PAH
Benzophenone[1]	50	3.15	119–61–9	Fixative for perfumes and soaps
beta-Sitosterol[1]	500	9.65	83–46–5	Plant sterol
beta-Stigmastanol[1]	500	9.73	19466–47–8	Herbivore fecal indicator (digestion of sitosterol)
Bisphenol A[10]	50	3.64	80–05–7	FR, manuf. polycarbonate resins, antioxidant
Bromacil[1]	500	1.68	314–40–9	H (GUP), >80% noncrop usage on grass/brush
Camphor[1]	50	3.04	76–22–2	Flavor, odorant, ointments.
Carbazole[1]	50	3.23	86–74–8	I, manuf. dyes, explosives, and lubricants
Chlorpyrifos [1]	50	4.66	2921–88–2	I, historically for domestic pest and termite control
Cholesterol[1]	250	8.74	57–88–5	Often a fecal indicator, also a plant sterol
Diazinon [1]	50	3.86	333–41–5	I, > 40% nonagricultural usage, ants, flies
d-Limonene[1]	50	4.83	5989–27–5	F, antimicrobial, antiviral, fragrance in aerosols
Fluoranthene[1]	50	4.93	206–44–0	CP, in coal tar, asphalt (traces in gasoline or diesel fuel)
Hexahydrohexamethyl-cyclopenta-benzopyran (galaxolide) [1]	50	6.26	1222–05–5	Musk fragrance
Indole[1]	100	2.05	120–72–9	Pesticide inert ingredient, fragrance in coffee
Isoborneol[1]	50	2.85	124–76–5	Fragrance in perfumery, in disinfectants
Isophorone[1]	50	2.62	78–59–1	Solvent for lacquer, plastic, oil, silicon, resin
Isopropylbenzene (cumene) [1]	100	3.45	98–82–8	Manuf. phenol/acetone, fuels and paint thinner
Isoquinoline[1]	100	2.14	119–65–3	Flavors and fragrances
Menthol[1]	50	3.38	89–78–1	Cigarettes, cough drops, liniment, mouthwash
Metolachlor[1]	50	3.24	51218–45–2	H (GUP), indicator of agricultural drainage
N,N-diethyl-*meta*-toluamide[1]	100	2.26	134–62–3	I, urban uses, mosquito repellent
Naphthalene [1]	50	3.17	91–20–3	Fumigant, moth repellent, component (10%) of gasoline
p-Cresol (4-Methylphenol) [1]	250	2.06	106–44–5	Disinfectant

Phenanthrene [1]	50	4.35	85–01–8	CP, manuf. explosives, in tar, diesel fuel, or crude oil
Phenol [1]	50	1.51	108–95–2	Disinfectant, manuf several products, leachate
Prometon[1]	50	3.57	1610–18–0	H (non-crop only), applied prior to blacktop
Pyrene [1]	50	4.93	129–00–0	CP , In coal tar, asphalt (traces in gasoline or diesel fuel)
Tributyl phosphate[1]	50	3.82	126–73–8	Antifoaming agent, flame retardant
Triclosan[1]	50	4.66	3380–34–5	Disinfectant, antimicrobial
Triphenyl phosphate[1]	50	4.70	115–86–6	FR, plasticizer, resin, wax, finish, roofing paper
Tris(2-butoxyethyl) phosphate[1]	150	3.00	78–51–3	Flame retardant
Tris(2-chloroethyl) phosphate [1]	100	1.63	115–96–8	Plasticizer, flame retardant
Tris(dichloroisopropyl) phosphate[1]	100	3.65	13674–87–8	Flame retardant
Bisphenol A-d3, (percent)	--	--	--	Surrogate standard
Caffeine-13C, (percent)	--	--	--	Surrogate standard
Decafluorobiphenyl, (percent)	--	--	--	Surrogate standard
Fluoranthene-d10, (percent) [1]	--	--	--	Surrogate standard
Hormones Analyzed in Bottom Sediment at the USGS National Water Quality Laboratory (ng/g)				
11-Ketotestosterone [1]	0.26	--	--	Reproductive hormone
17-alpha-Estradiol [1]	0.1	--	--	Reproductive hormone
17-beta-Estradiol (E2) [1]	0.1	--	--	Reproductive hormone
17-alpha-Ethynylestradiol (EE2) [1]	0.1	--	--	Ovulation inhibitor
Norethindrone [1]	0.1	--	--	Ovulation inhibitor
4-Androstene-3,17-dione [1]	0.1	--	--	Anabolic agent and natural steroid
cis-Androsterone [1]	0.1	--	--	Urinary steroid
Cholesterol [1]	250	--	--	Plant/animal steroid
3-beta-Coprostanol [1]	250	--	--	Fecal steroid
Dihydrotestosterone [1]	0.1	--	--	Metabolite of testosterone
Bisphenol A [1]	12	--	--	Plastic component
Epitestosterone [1]	0.5	--	--	Form of testosterone
Equilenin [1]	0.26	--	--	Hormone replacement
Equilin [1]	0.5	--	--	Hormone replacement
Estriol [1]	0.26	--	--	Reproductive hormone
Estrone [1]	0.1	--	--	Reproductive hormone
Mestranol [1]	0.1	--	--	Ovulation inhibitor
Progesterone [1]	0.5	--	--	Reproductive hormone
trans-Diethylstilbestrol [1]	0.1	--	--	Synthetic metabolic intermediate of diethylstilbestrol

Testosterone [1]	0.1	--	--	Reproductive hormone
Testosterone-2,2,4,6,6-d5	--	--	--	Surrogate Standard
17-alpha-Ethynylestradiol-2,4,16,16-d4	--	--	--	Surrogate Standard
Mestranol-2,4,16,16-d4	--	--	--	Surrogate Standard
Dihydrotestosterone-1,2,4,5a-d4	--	--	--	Surrogate Standard
Bisphenol-A-d16	--	--	--	Surrogate Standard
4-Androstene-3,17-dione-2,2,4,6,6,16,16-d7	--	--	--	Surrogate Standard
Norethindrone-2,2,4,6,6,10-d6	--	--	--	Surrogate Standard
Cholesterol-d7	--	--	--	Surrogate Standard
Progesterone-2,2,4,6,6,17a,21,21,21-d9	--	--	--	Surrogate Standard
Estriol-2,4,17-d3	--	--	--	Surrogate Standard
Estrone-2,4,16,16-d4	--	--	--	Surrogate Standard
17-beta-Estradiol-d4	--	--	--	Surrogate Standard
trans-Diethyl-1,1,1',1'-d4-stilbesterol-3,3',5,5'-d4	--	--	--	Surrogate Standard

[1]Chemicals with and "E" following the number indicate a compound with low recovery, unstable instrument response, or reference standard prepared from a technical mixture for water analyses (Zaugg and others, 2006). Chemicals with an "e" following the number are estimated if the spike recovery or expected continuing calibration verification concentrations for each set of samples are not within control limits (Zaugg and others, 2006).

[2]Endocrine disrupting potential (EDP) from the following sources: Kime, 1998; Tremblay and Van der Kraak, 1998; EC-BKH, 2000; Nishihara and others, 2000; Global Water Research Coalition, 2003; Versonnen and others, 2003; Institute of Environmental Health, 2005; Korner and others, 2005; and Terasaki and others, 2005; Scheurs and others, 2004.

[3]Log K_{ow} is the octanol-water partition coefficient and is a measure of the equilibrium concentration of a compound between octanol and water. A high value indicates a compound that will preferentially partition into soil organic matter rather than water. It was calculated using the U.S. Environmental Protection Agency's exposure assessment tools and models (EPI-suite software, WSKOWWINTM version 1.40; U.S. Environmental Protection Agency, 2005b).

[4]This report contains Chemical Abstracts Services Registry Numbers (CASRN)®, which is a Registered Trademark of the American Chemical Society. A CASRN is a numeric identifier that can contain up to nine digits, divided by dashes into three parts. For example, 58–08–2 is the CASRN for caffeine. The online database provides a source for the latest registry number information: http://www.cas.org/index.html. Chemical Abstracts Services recommends the verification of the CASRNs through CAS Client Services℠.

[5]Sources are Kime, 1998; Tremblay and Van der Kraak, 1998; EC-BKH, 2000; Nishihara and others, 2000; Zaugg and others, 2007 Versonnen and others, 2003; Barber, Furlong, and others, 2003; Global Water Research Coalition, 2003; Institute of Environmental Health, 2005; Furlong and others, 2008; Korner and others, 2005; Terasaki and others, 2005.