

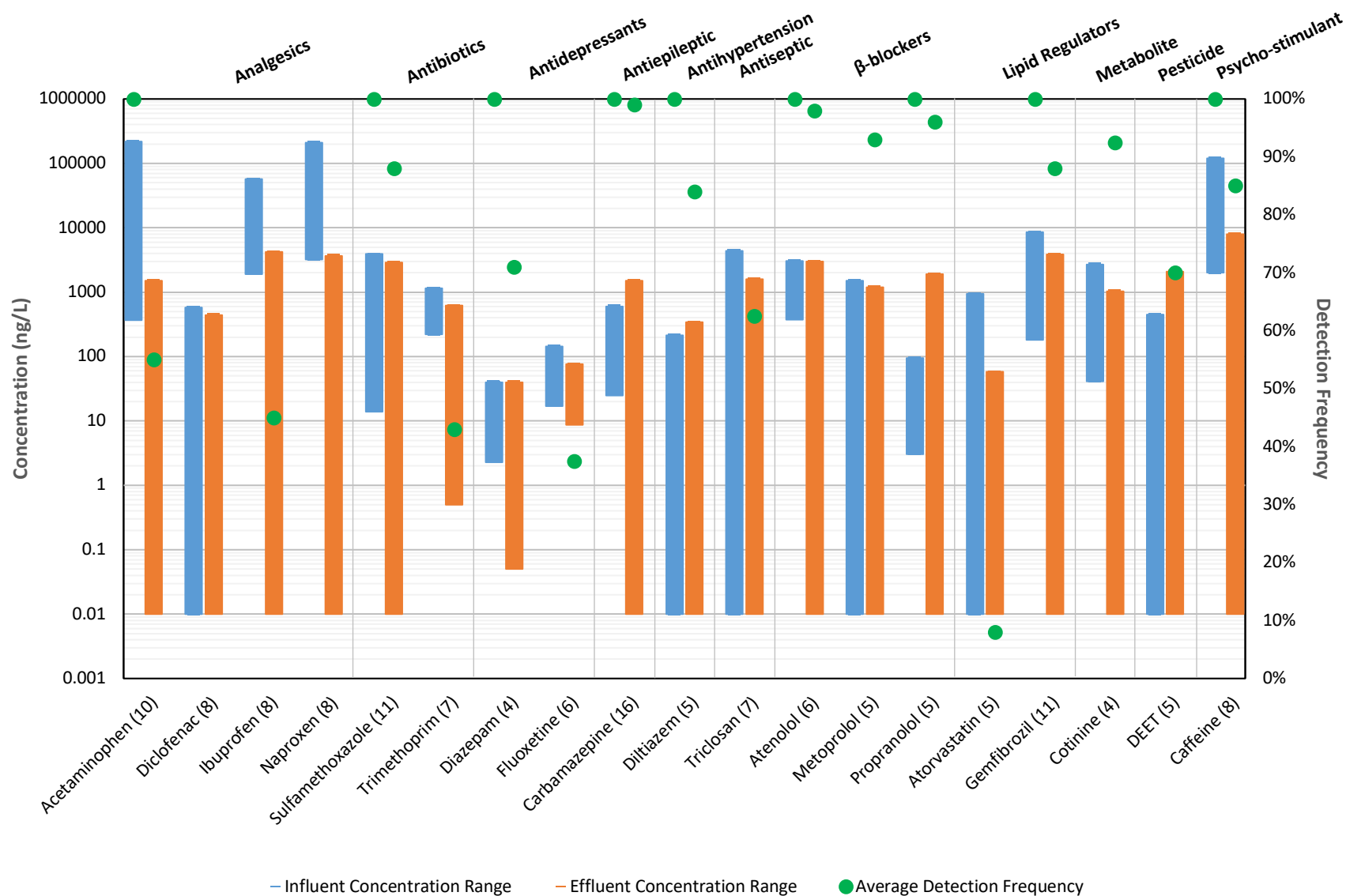


Figure S1. Concentration range of the most studied CECs in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

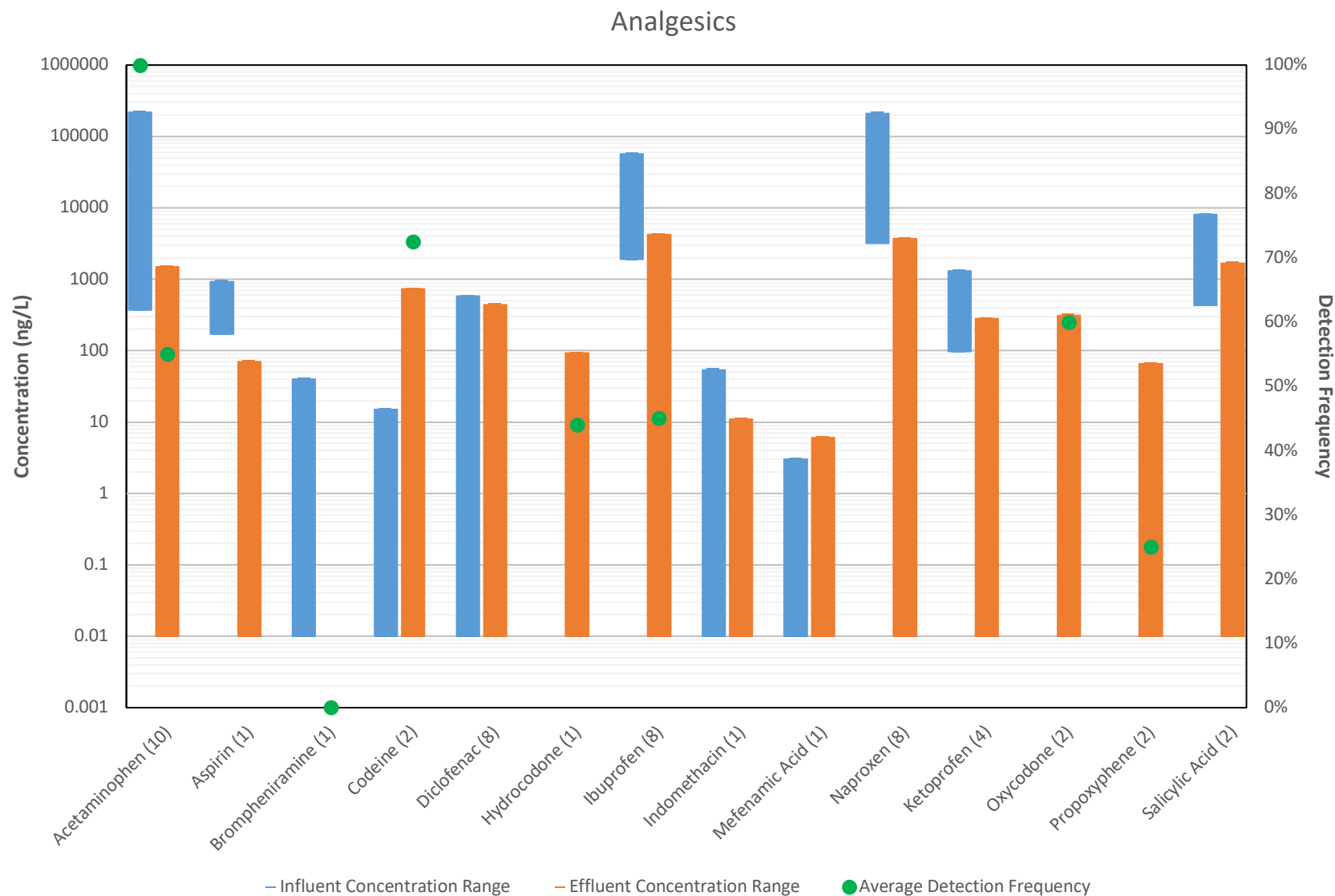


Figure S2. Concentration range of analgesics detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

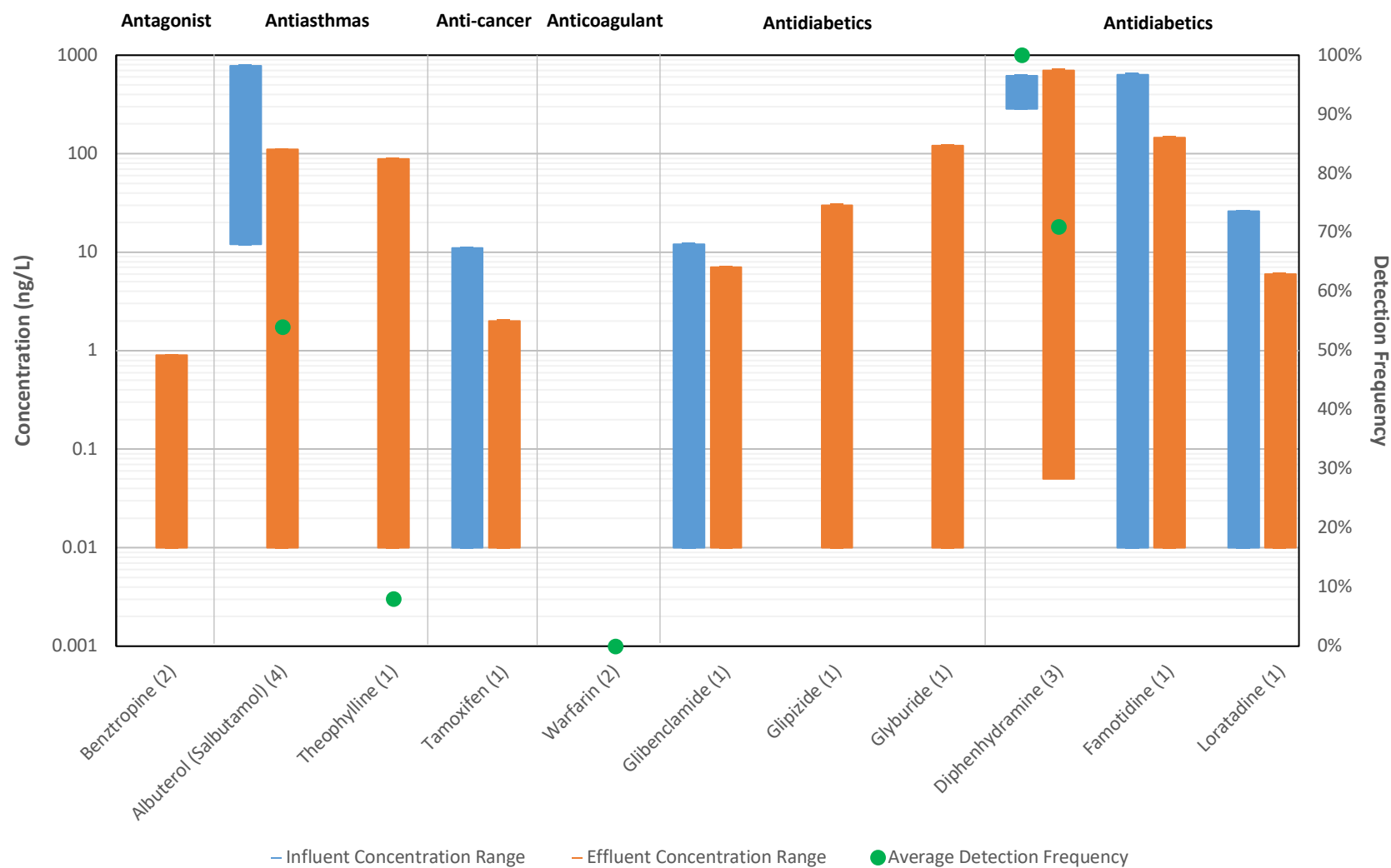


Figure S3. Concentration range of antagonist, antiasthmas, anti-cancer, anticoagulant, antidiabetics, and antidiabetics detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

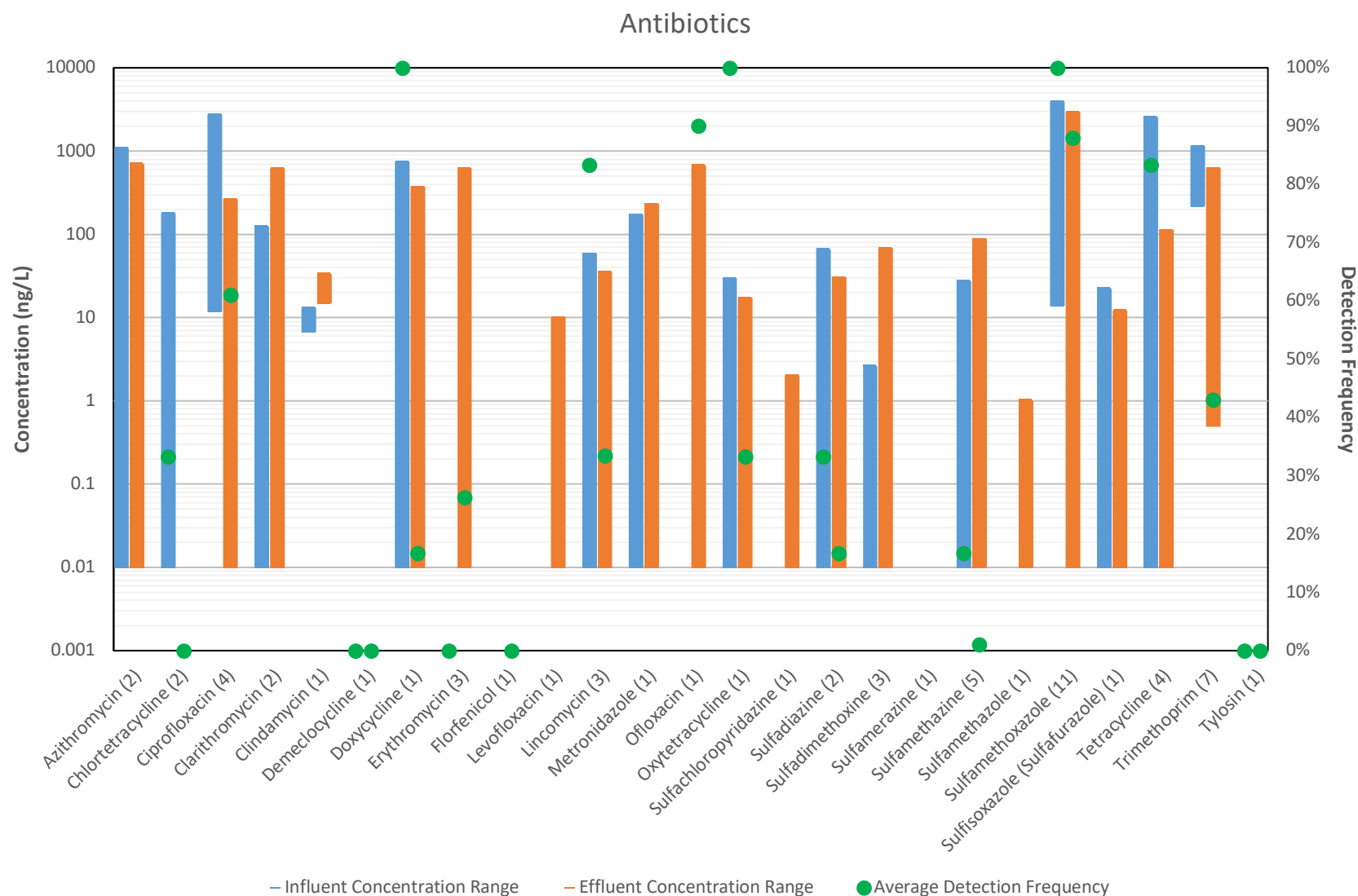


Figure S4. Concentration range of antibiotics detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

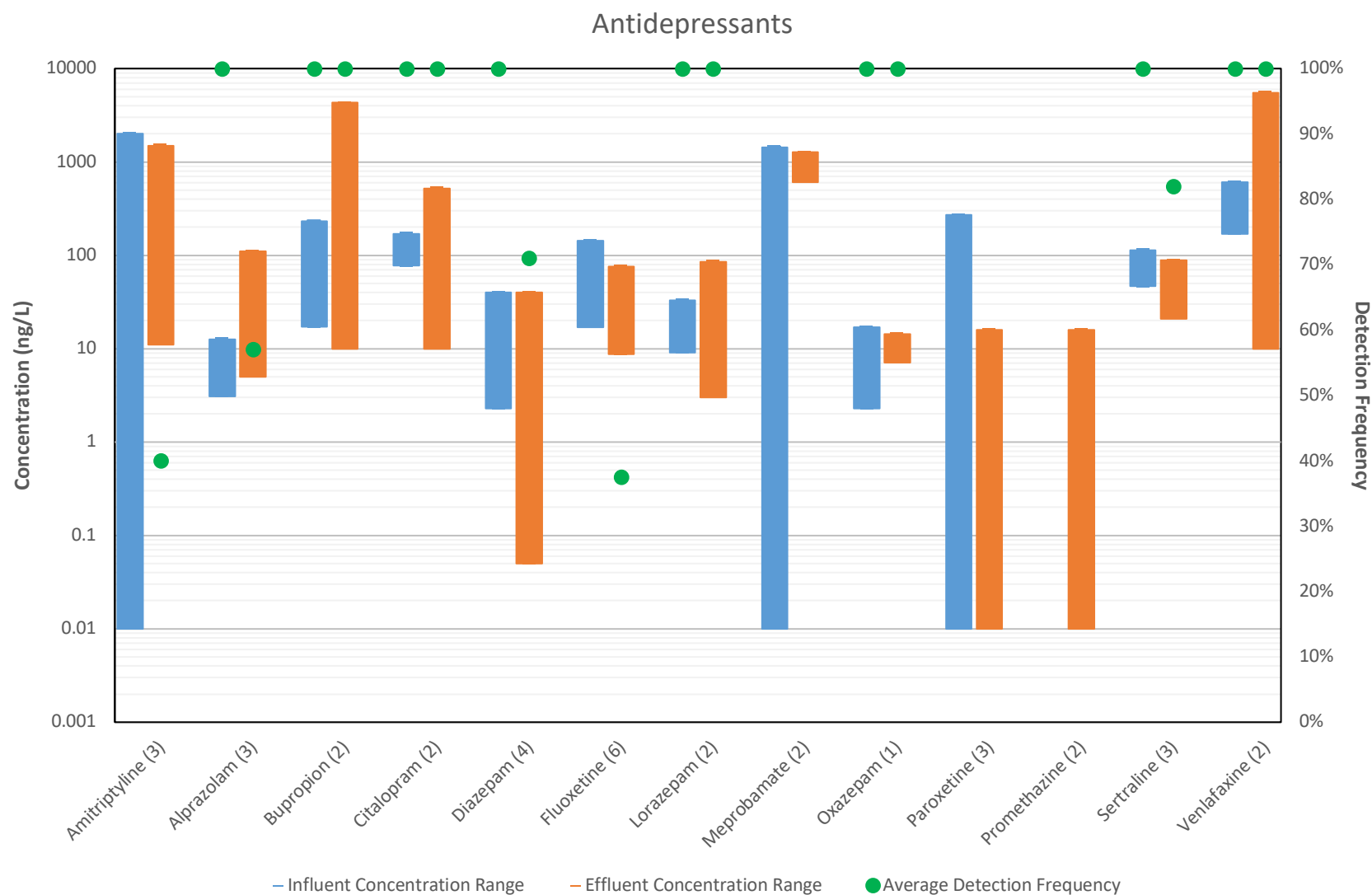


Figure S5. Concentration range of antidepressants detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

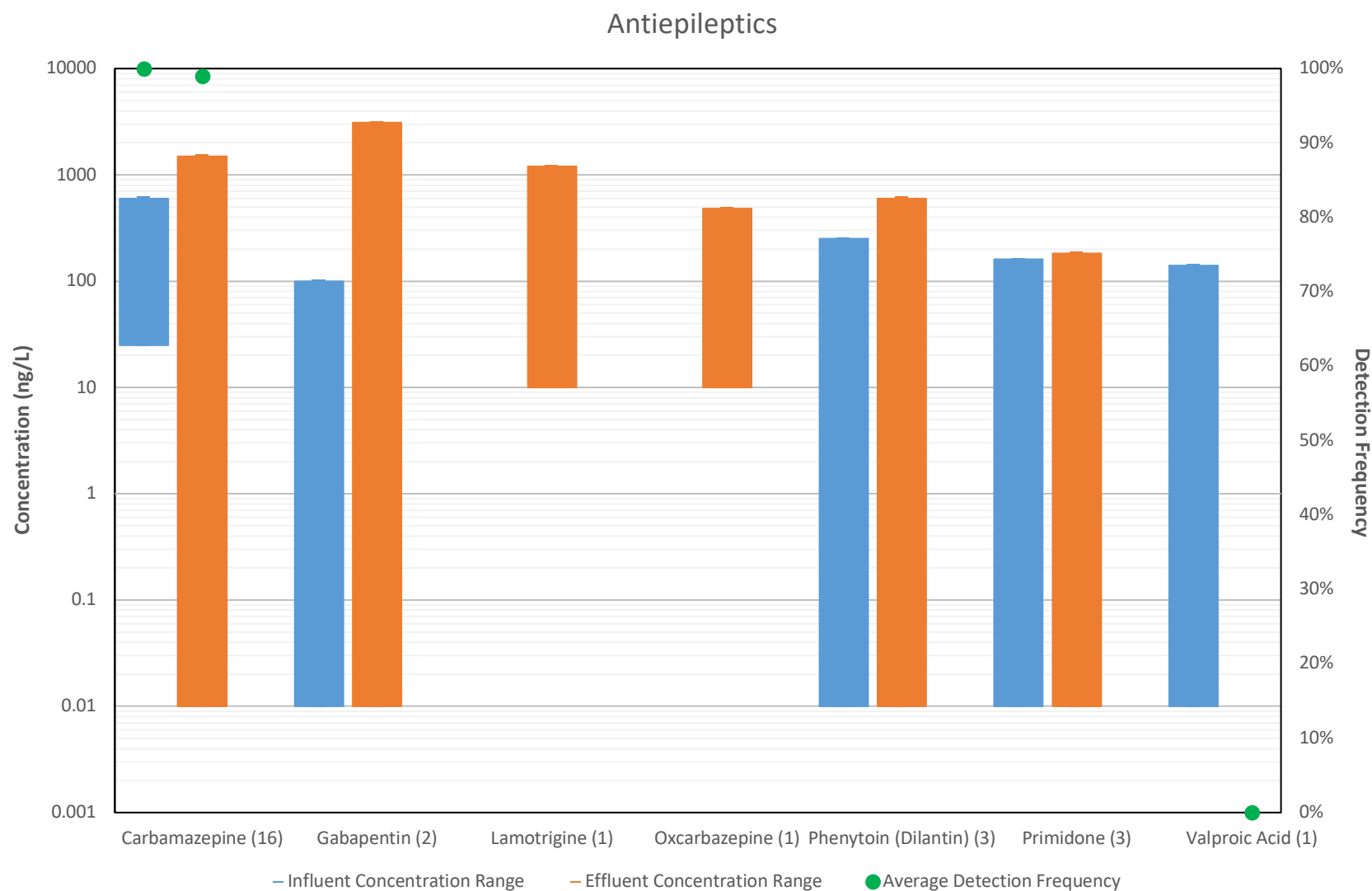


Figure S6. Concentration range of antiepileptics detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

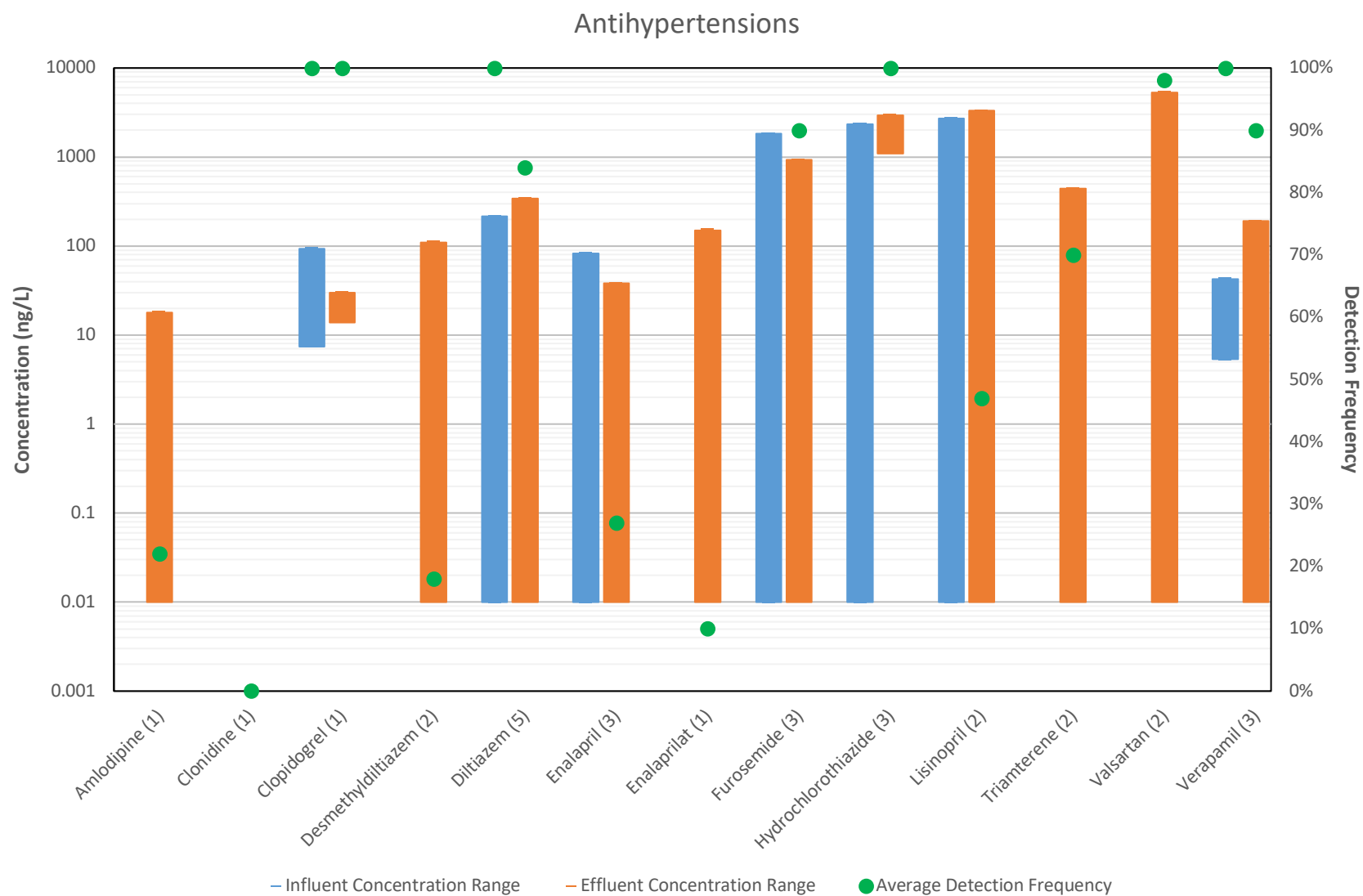


Figure S7. Concentration range of antihypertensions detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

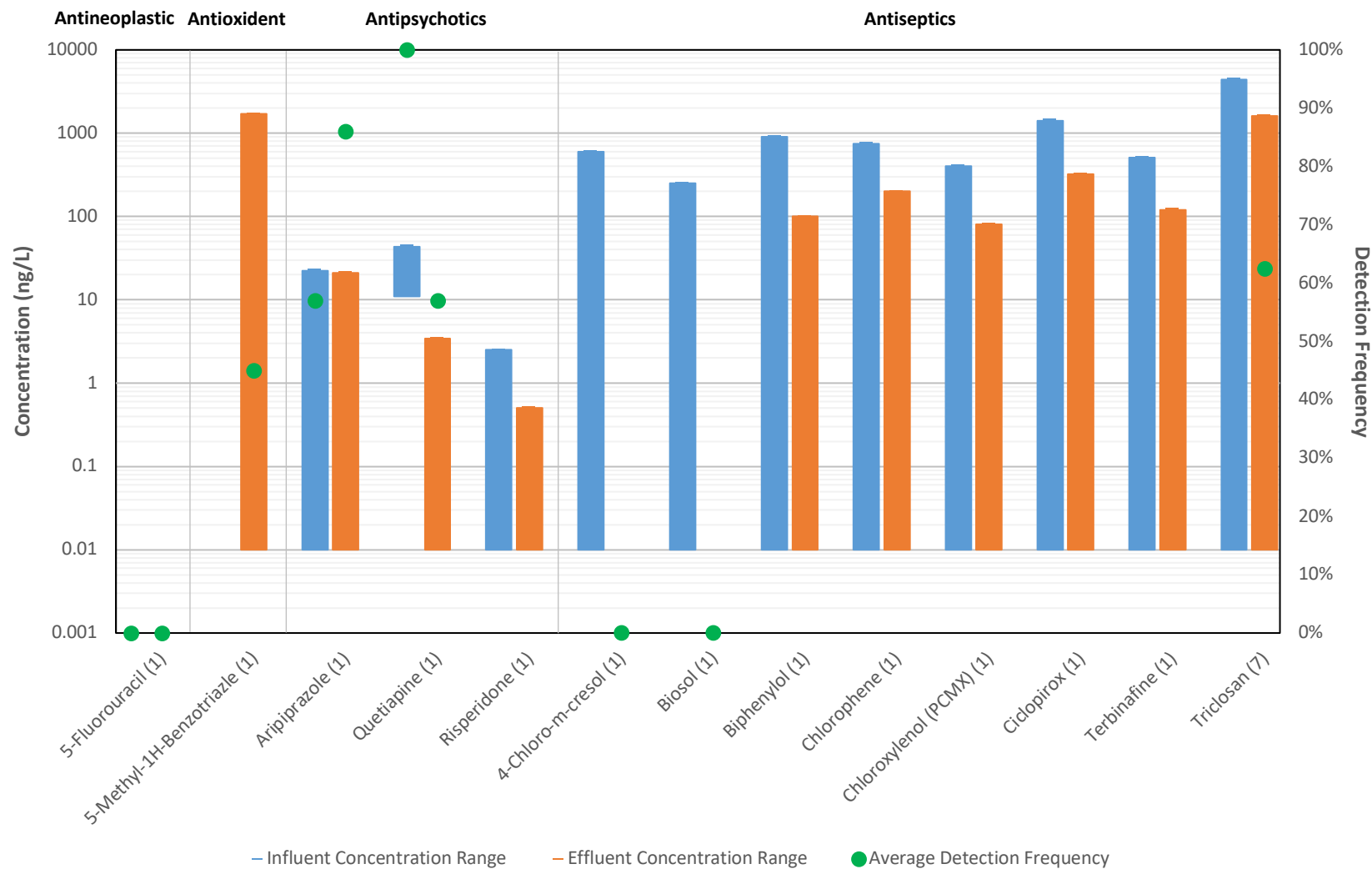


Figure S8. Concentration range of antineoplastic, antioxidant, antipsychotics, and antiseptics detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

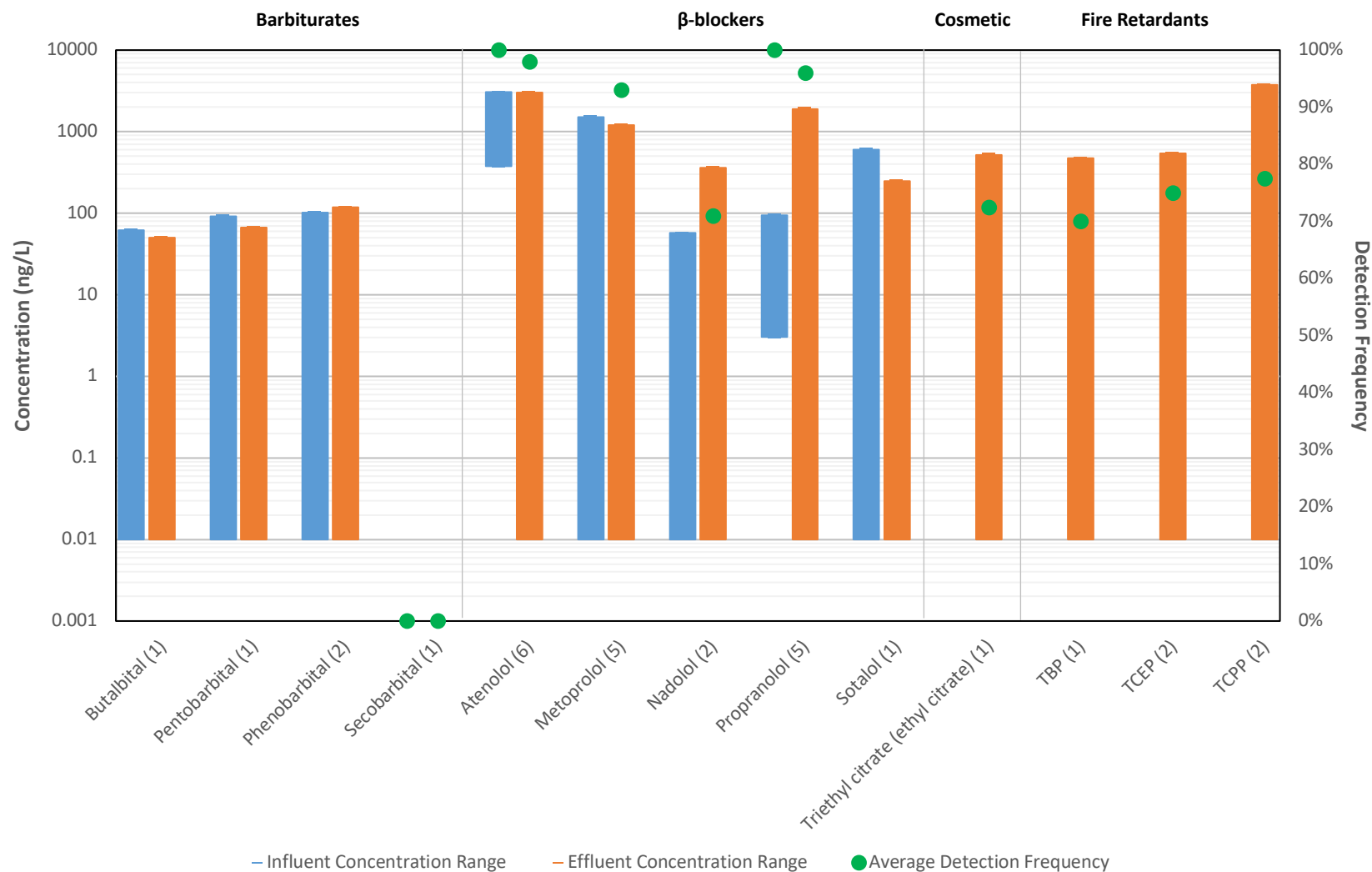


Figure S9. Concentration range of barbiturates, β -blockers, cosmetic, and fire retardants detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

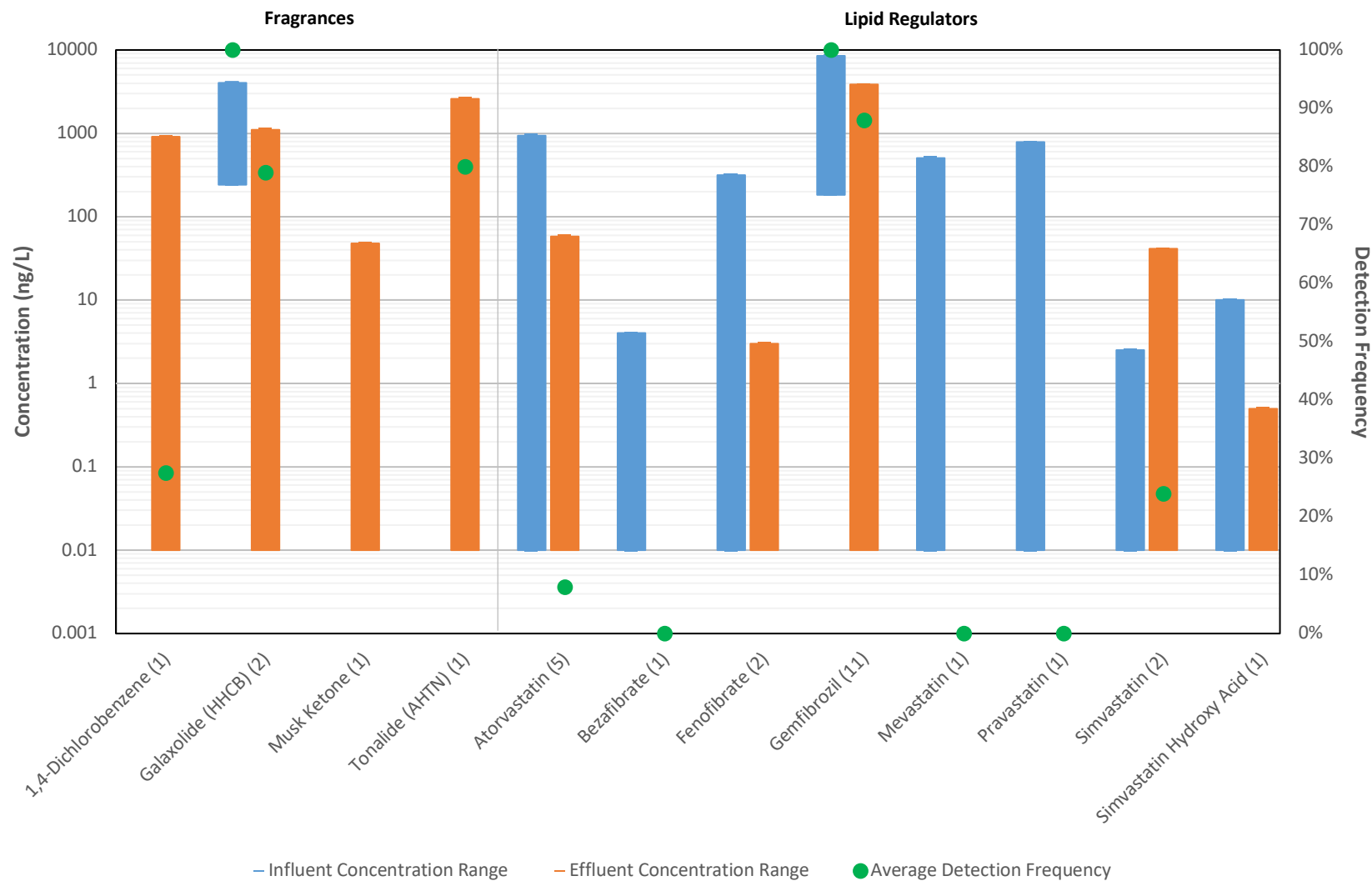


Figure S10. Concentration range of fragrances and lipid regulators detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

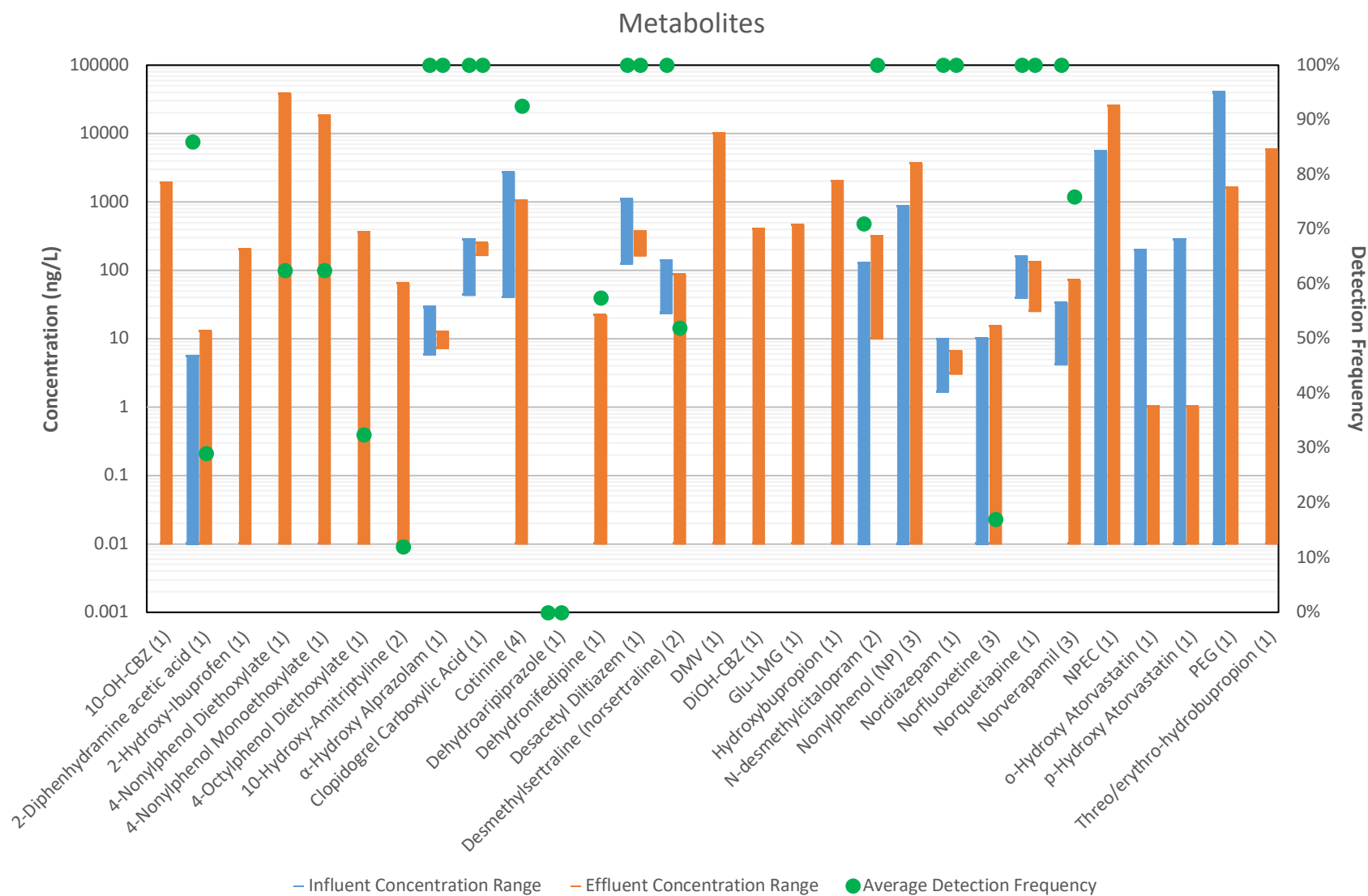


Figure S11. Concentration range of metabolites detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

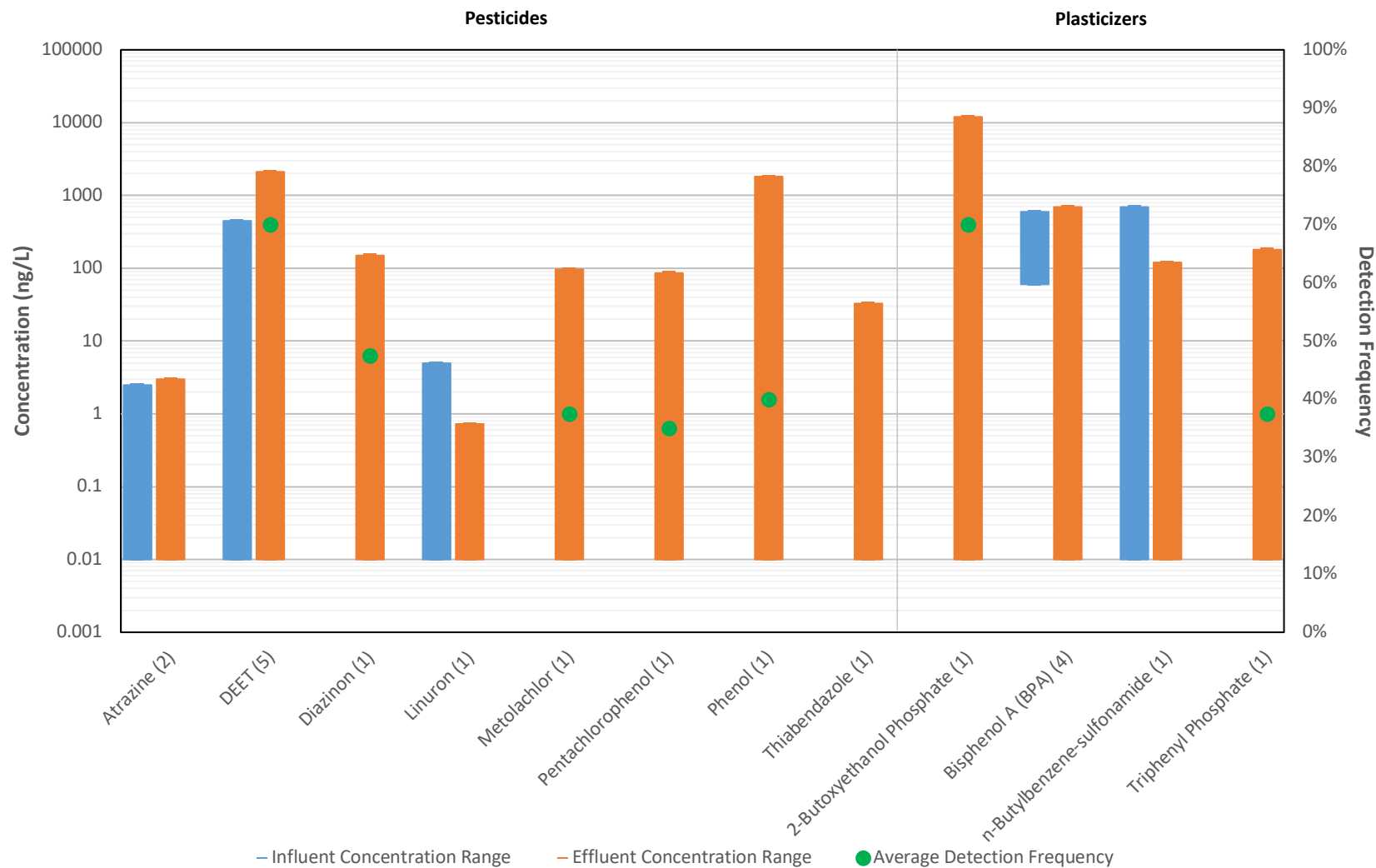


Figure S12. Concentration range of pesticides and plasticizers detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

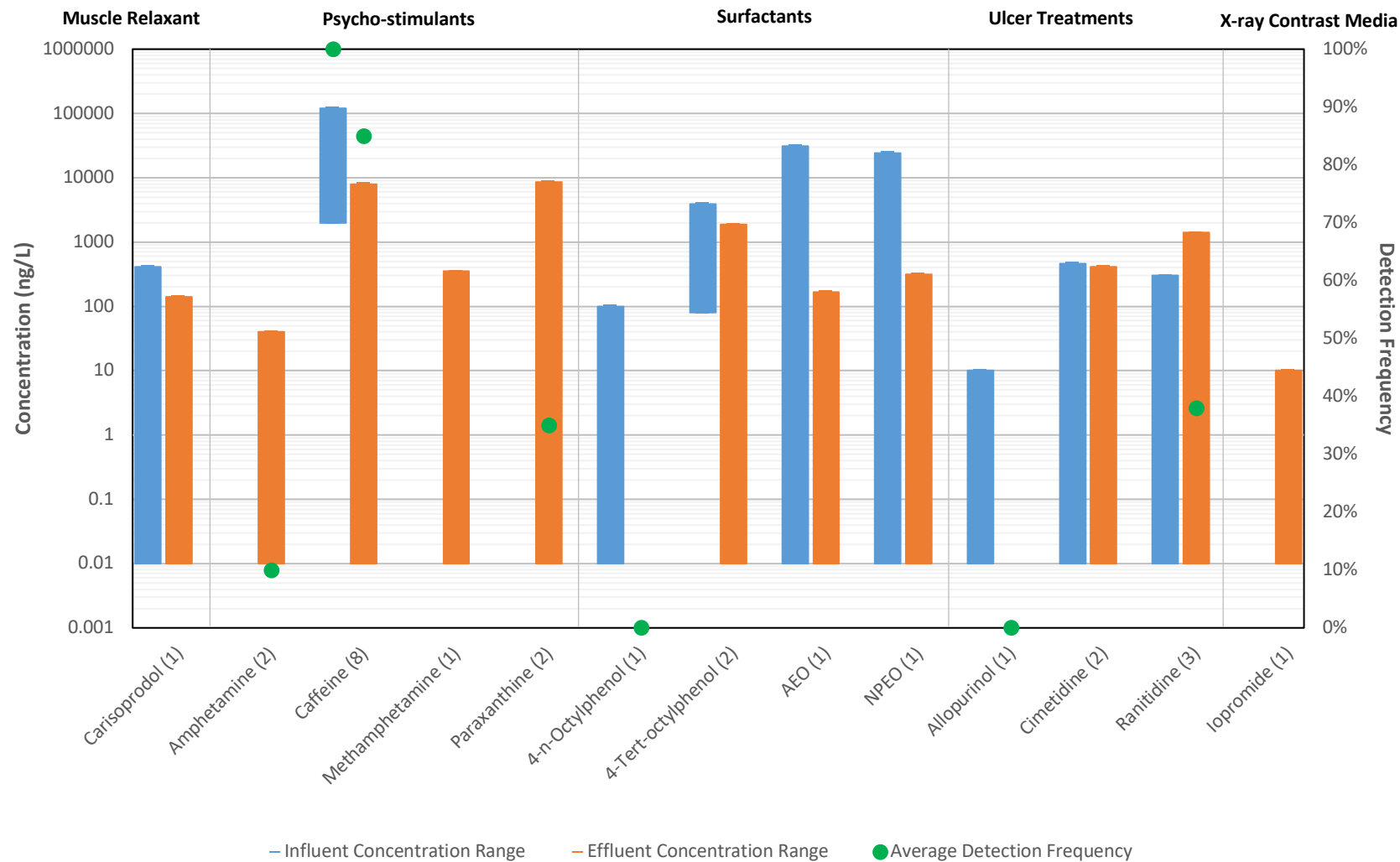


Figure S13. Concentration range of muscle relaxant, psycho-stimulants, surfactants, ulcer treatment, and x-ray contrast detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

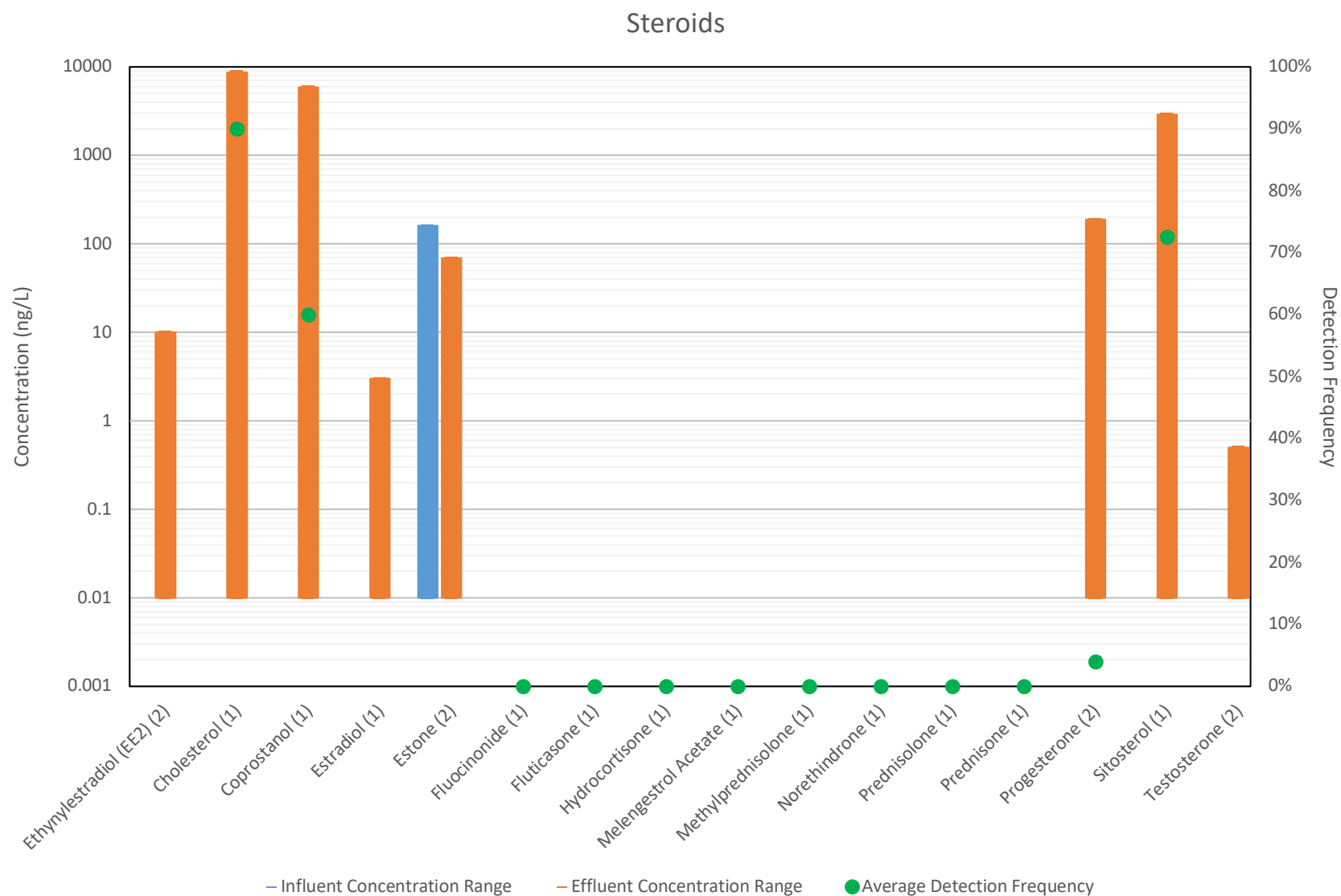


Figure S14. Concentration range of steroids detected in WWTP influents (blue bar) and effluents (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S5).

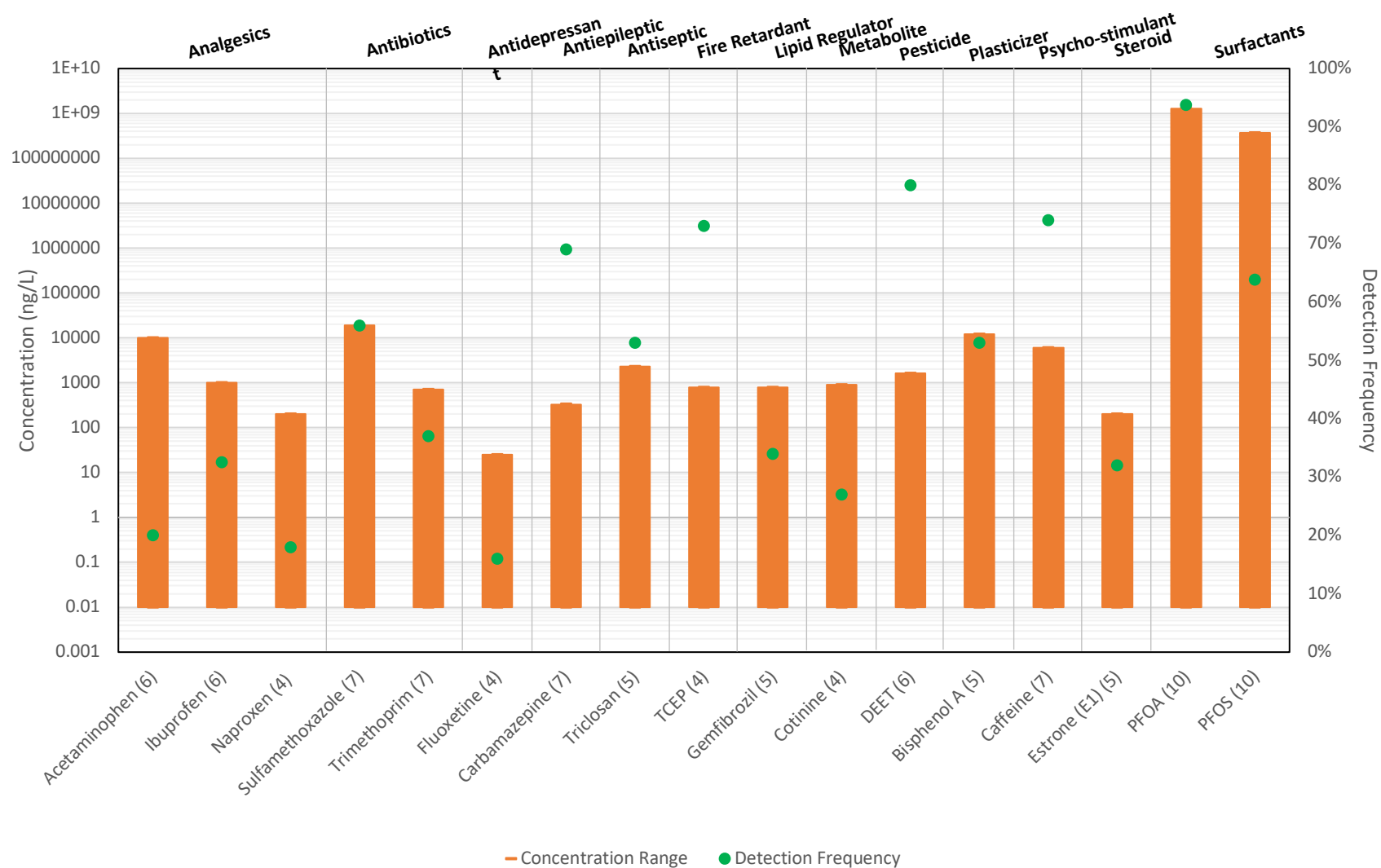


Figure S15. Concentration range of the most studied CECs in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

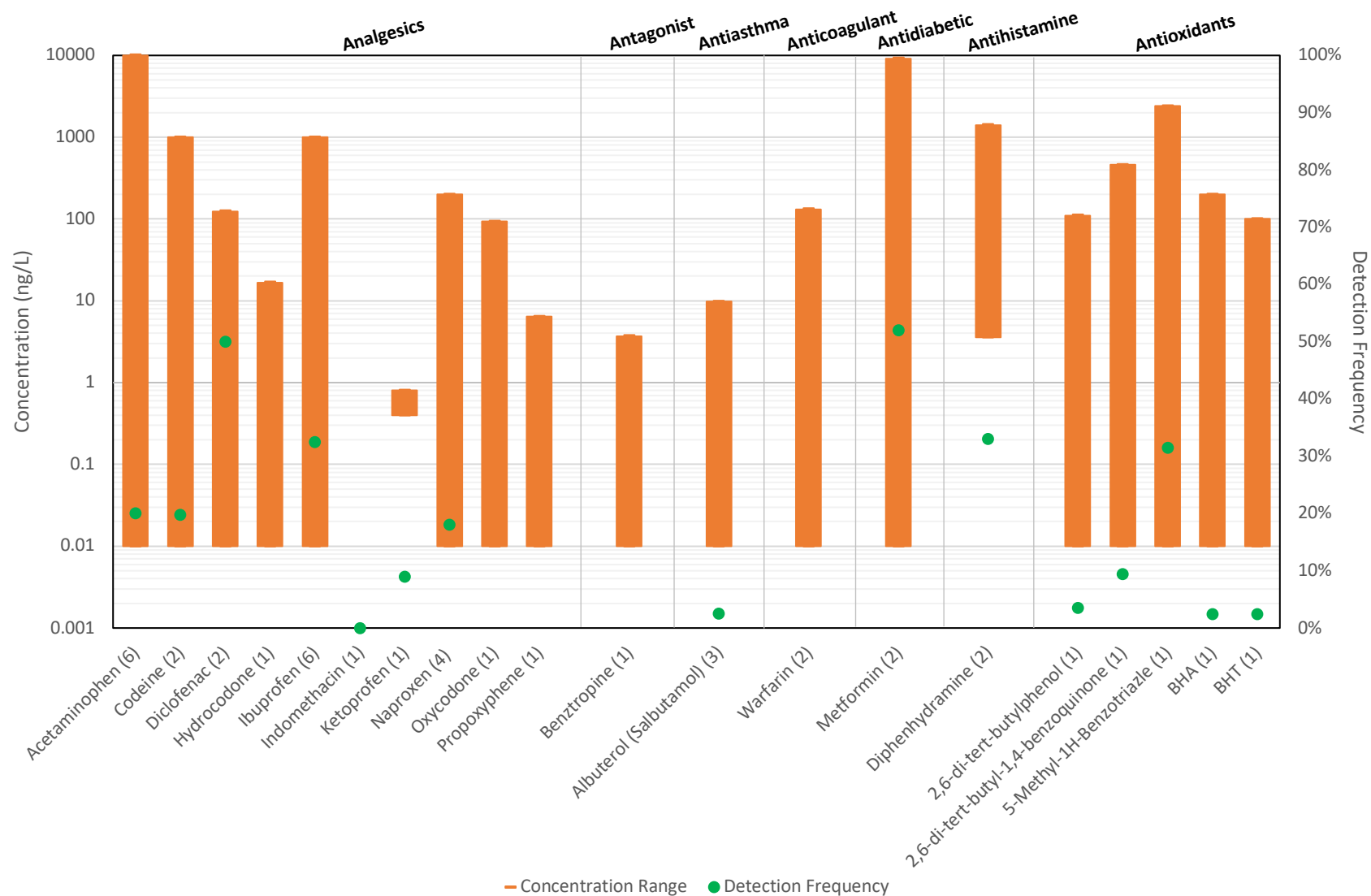


Figure S16. Concentration range of analgesics, antagonist, antiasthma, anticoagulant, antidiabetic, antihistamine, and antioxidants detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

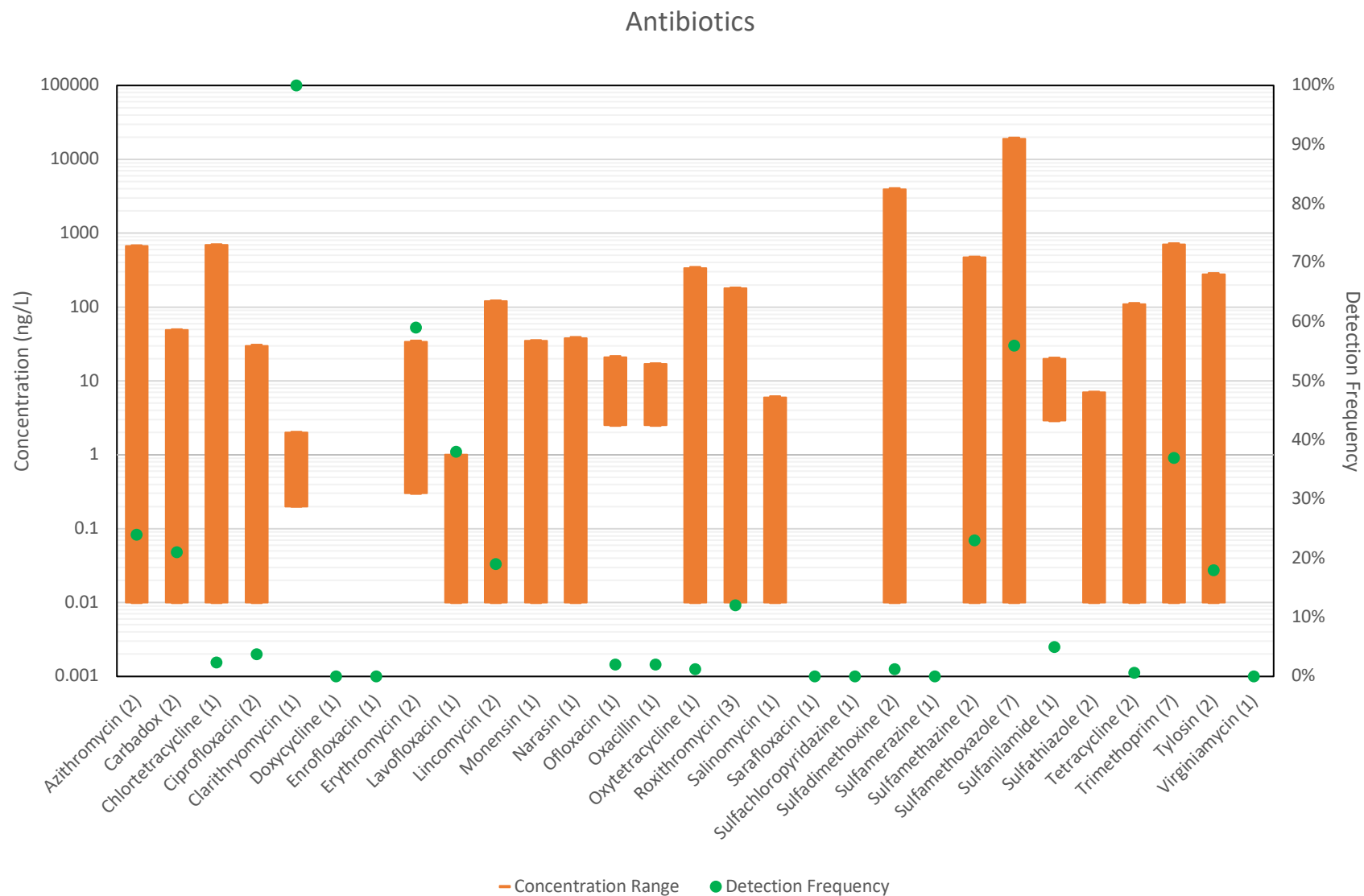


Figure S17. Concentration range of antibiotics detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

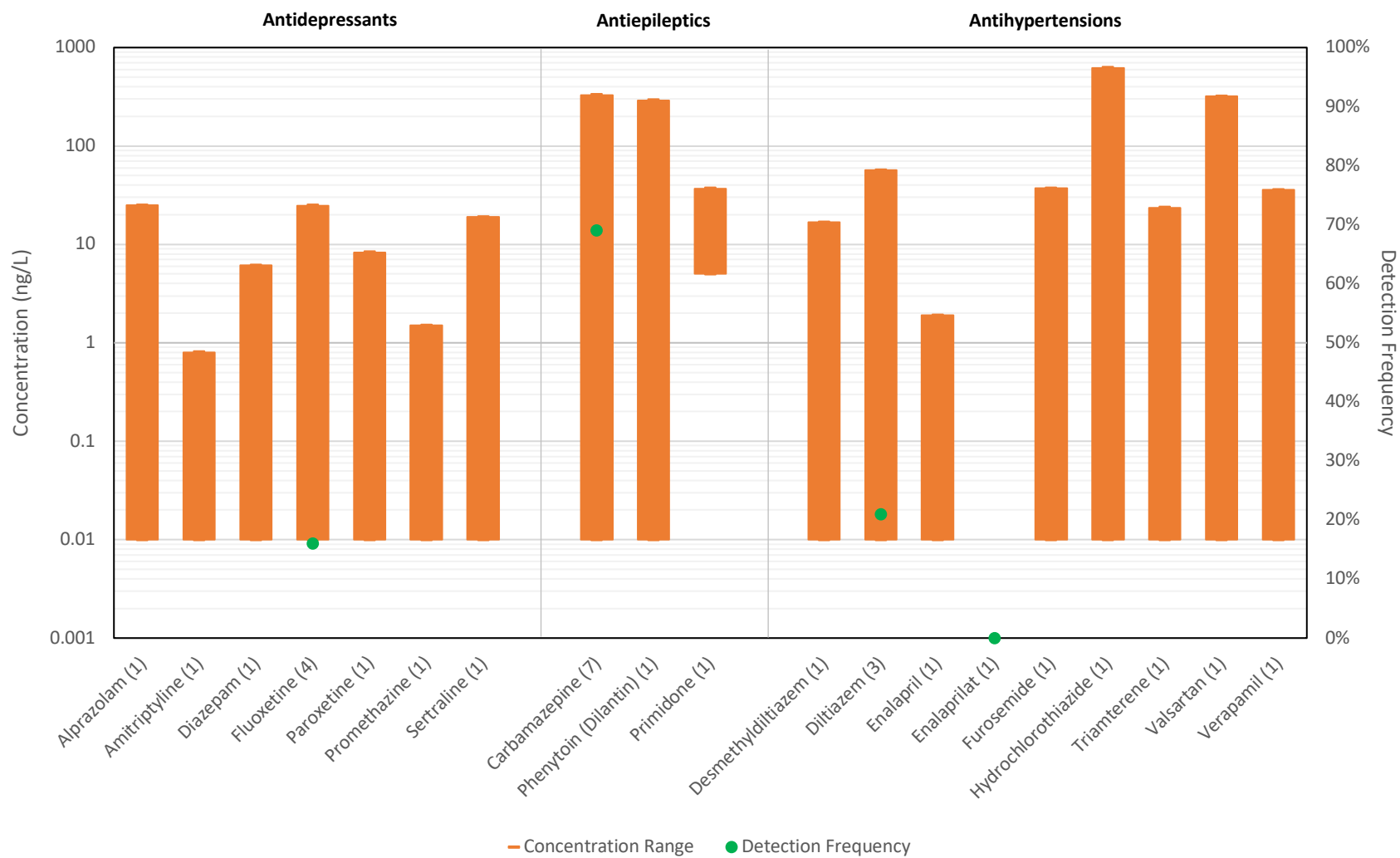


Figure S18. Concentration range of antidepressants, antiepileptics, and antihypertensives detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

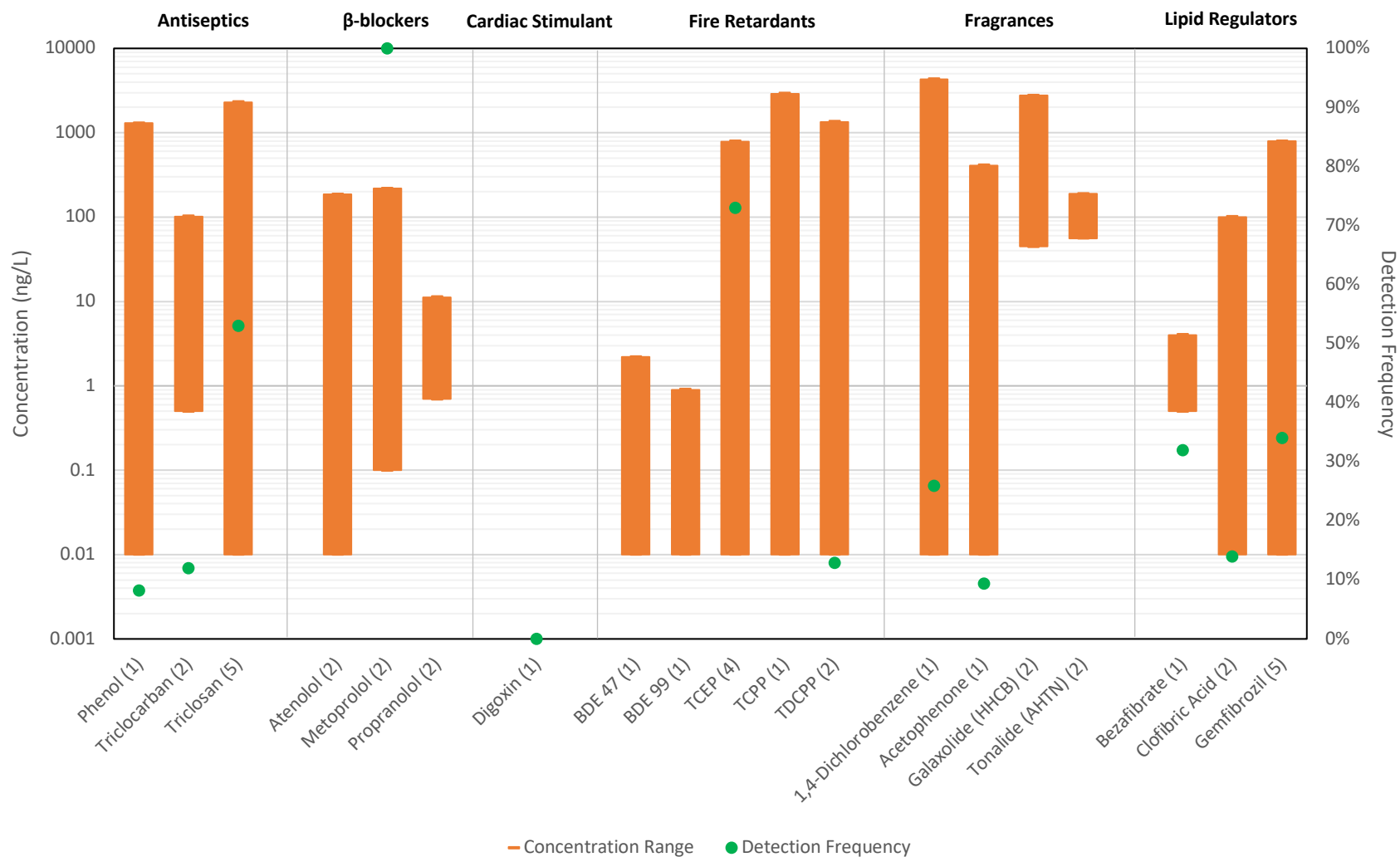


Figure S19. Concentration range of antiseptics, β -blockers, cardiac stimulant, fire retardants, fragrances, and lipid regulators detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

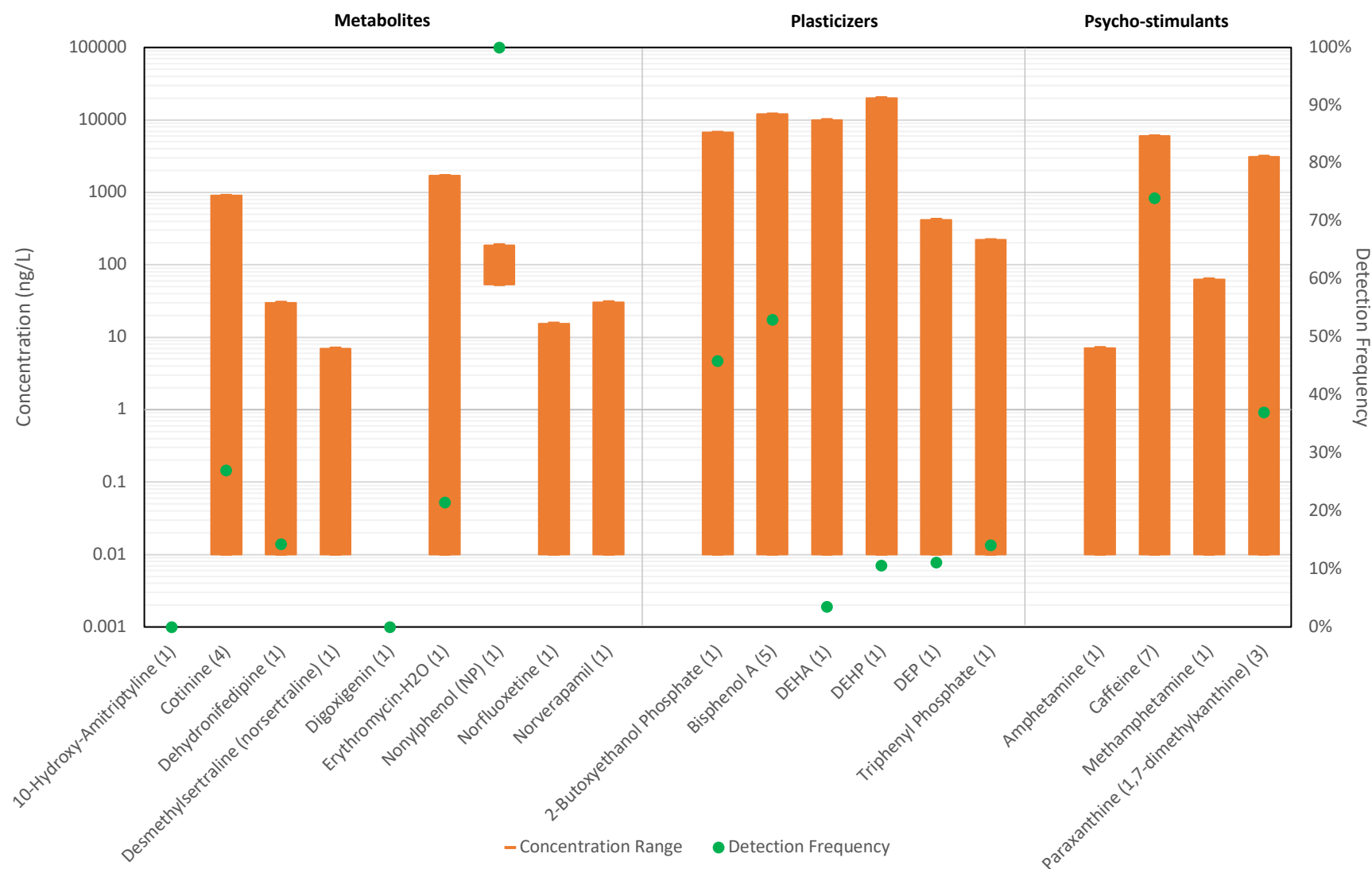


Figure S20. Concentration range of metabolites, plasticizers, and psycho-stimulants detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

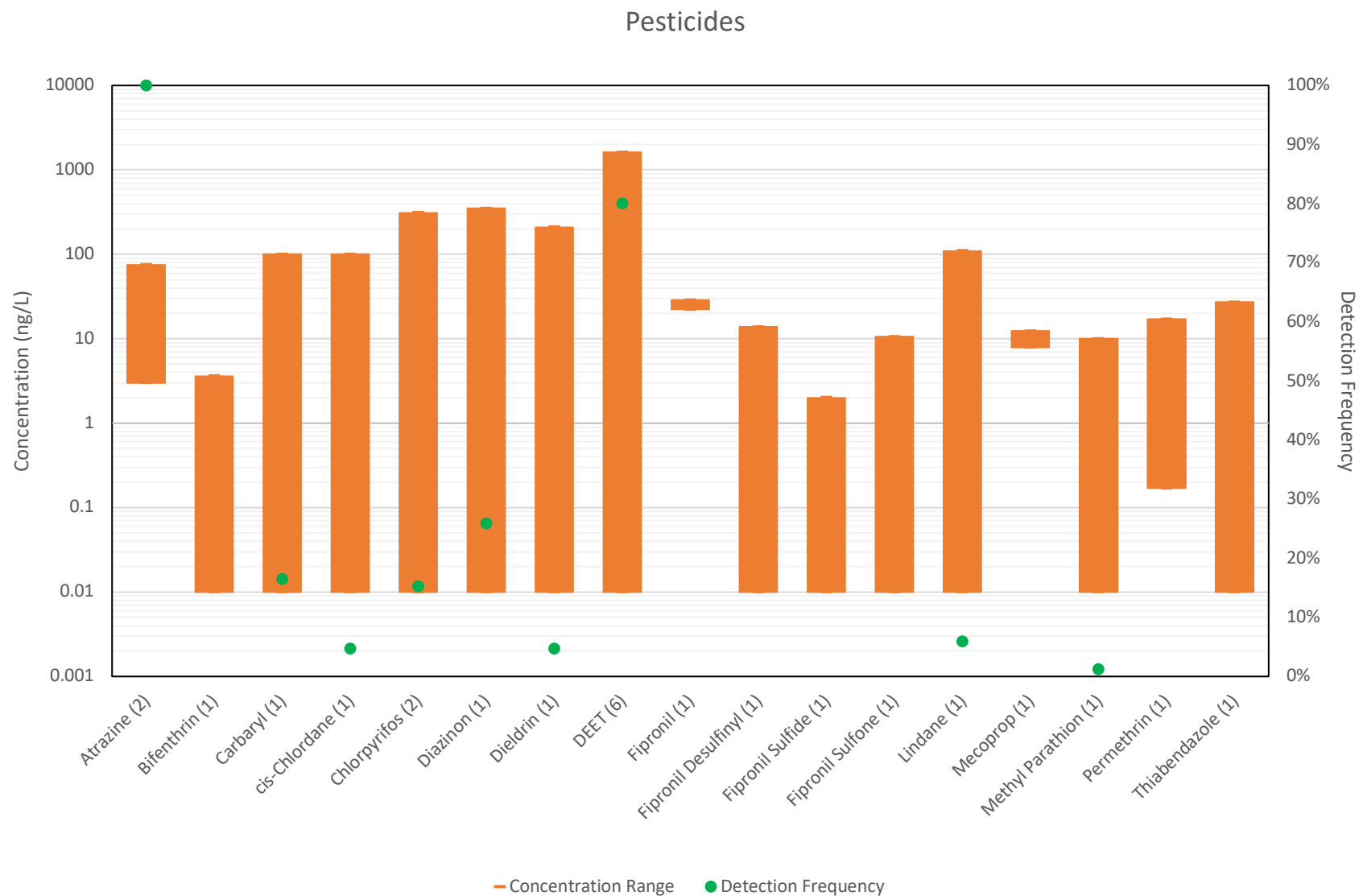


Figure S21. Concentration range of pesticides detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

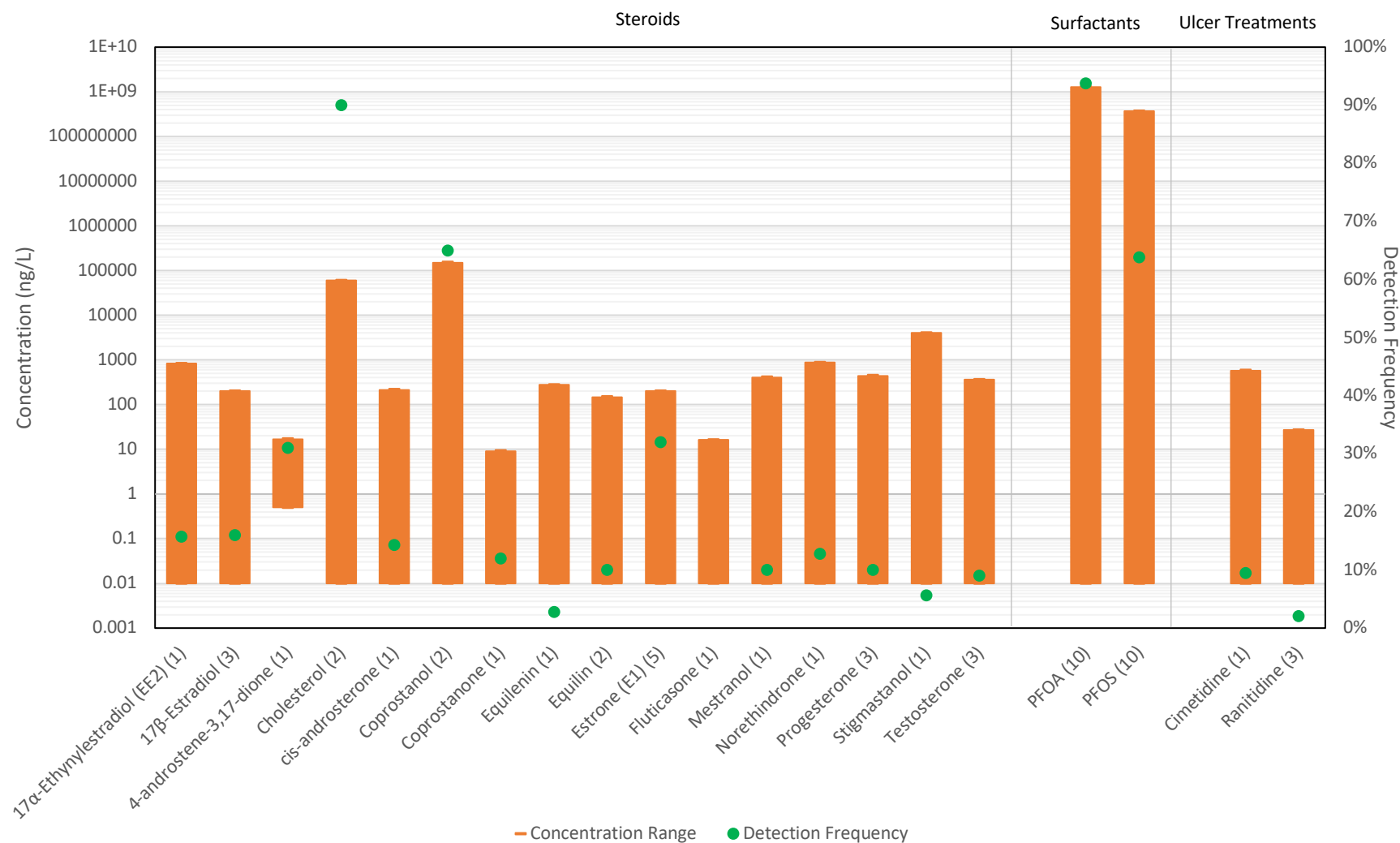


Figure S22. Concentration range of steroids and ulcer treatments detected in surface water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S6).

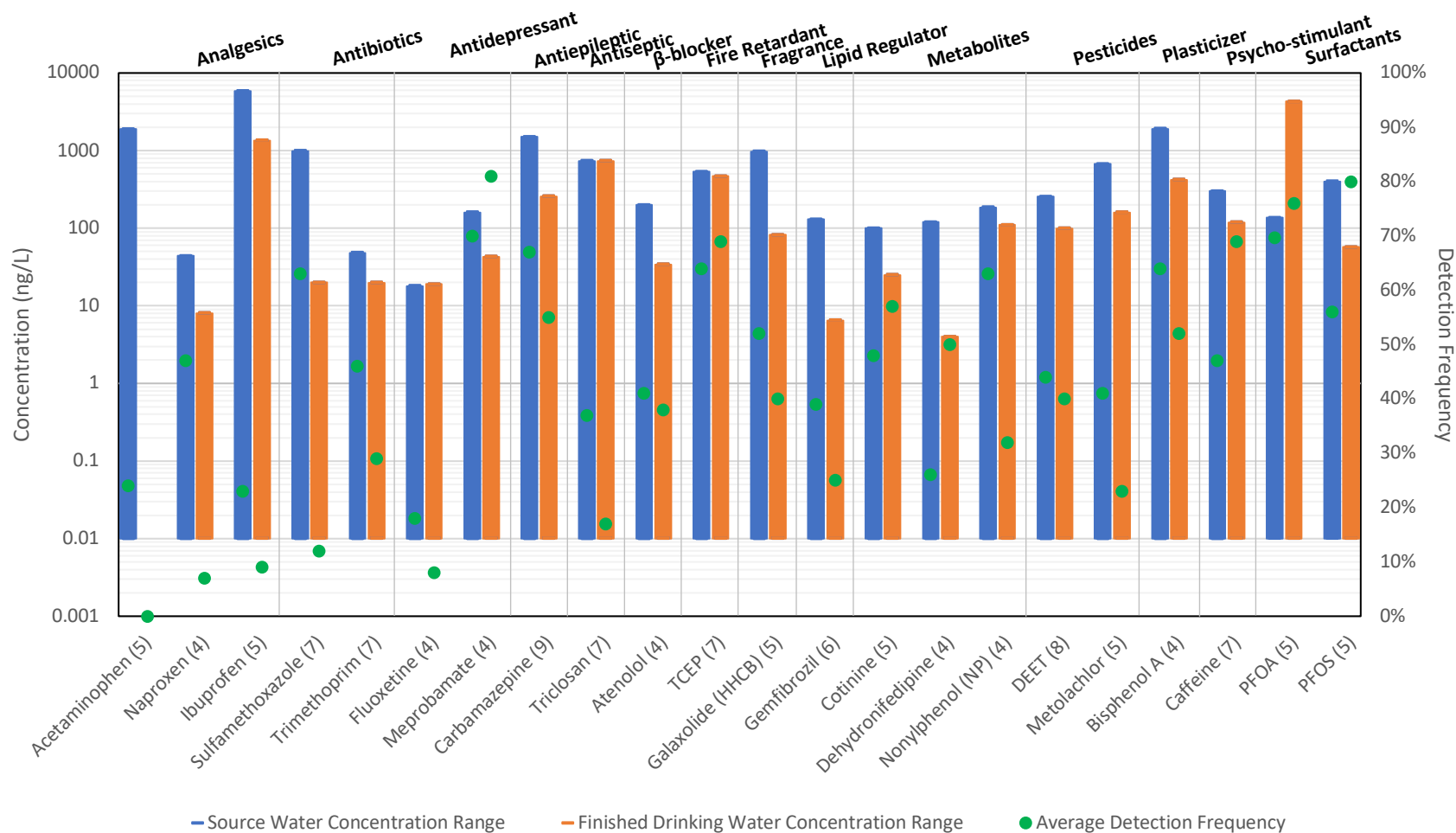


Figure S23. Concentration range of the most studied CECs in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

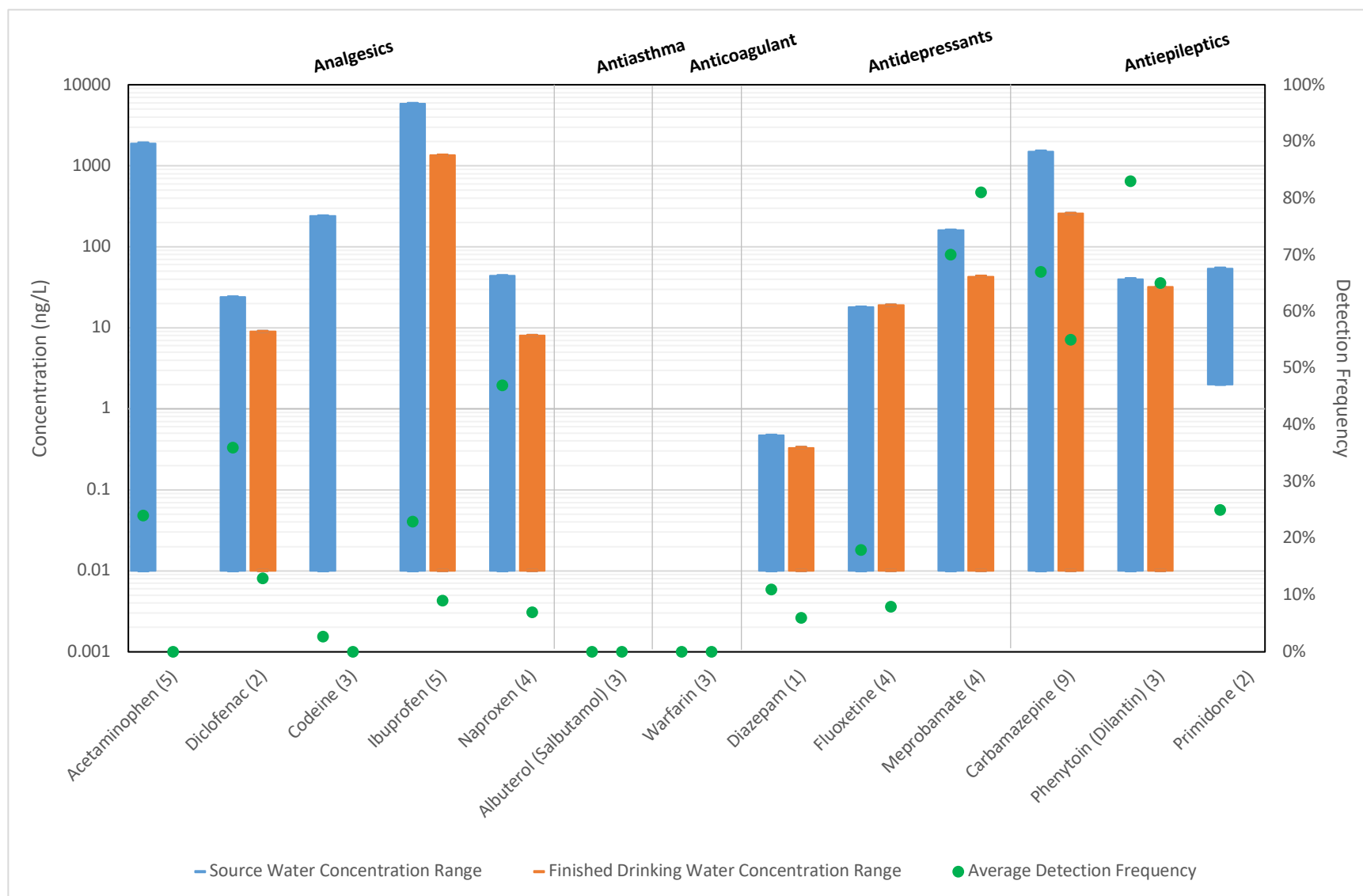


Figure S24. Concentration range of analgesics, antiasthma, anticoagulant, antidepressants, and antiepileptics detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

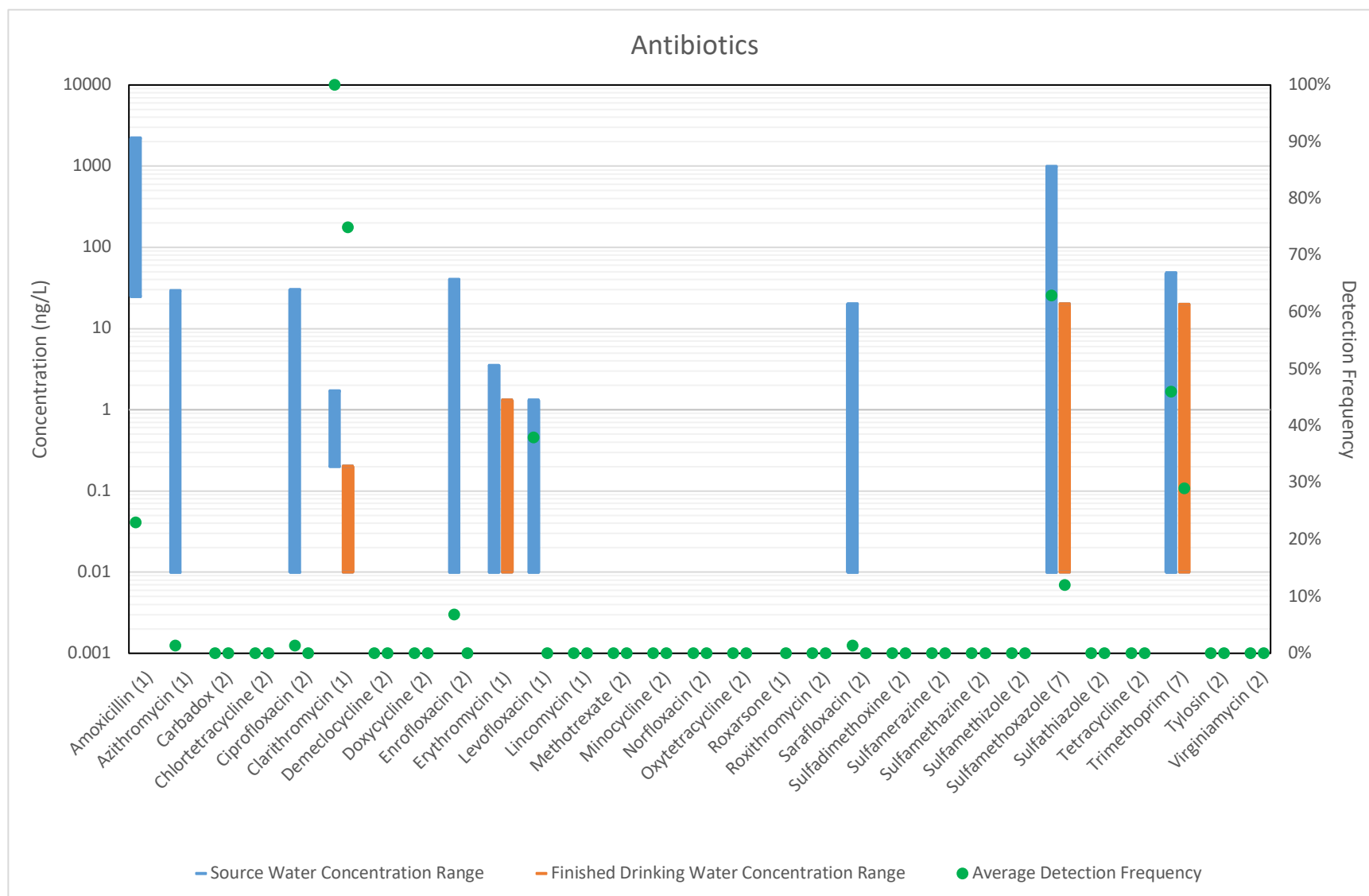


Figure S25. Concentration range of antibiotics detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

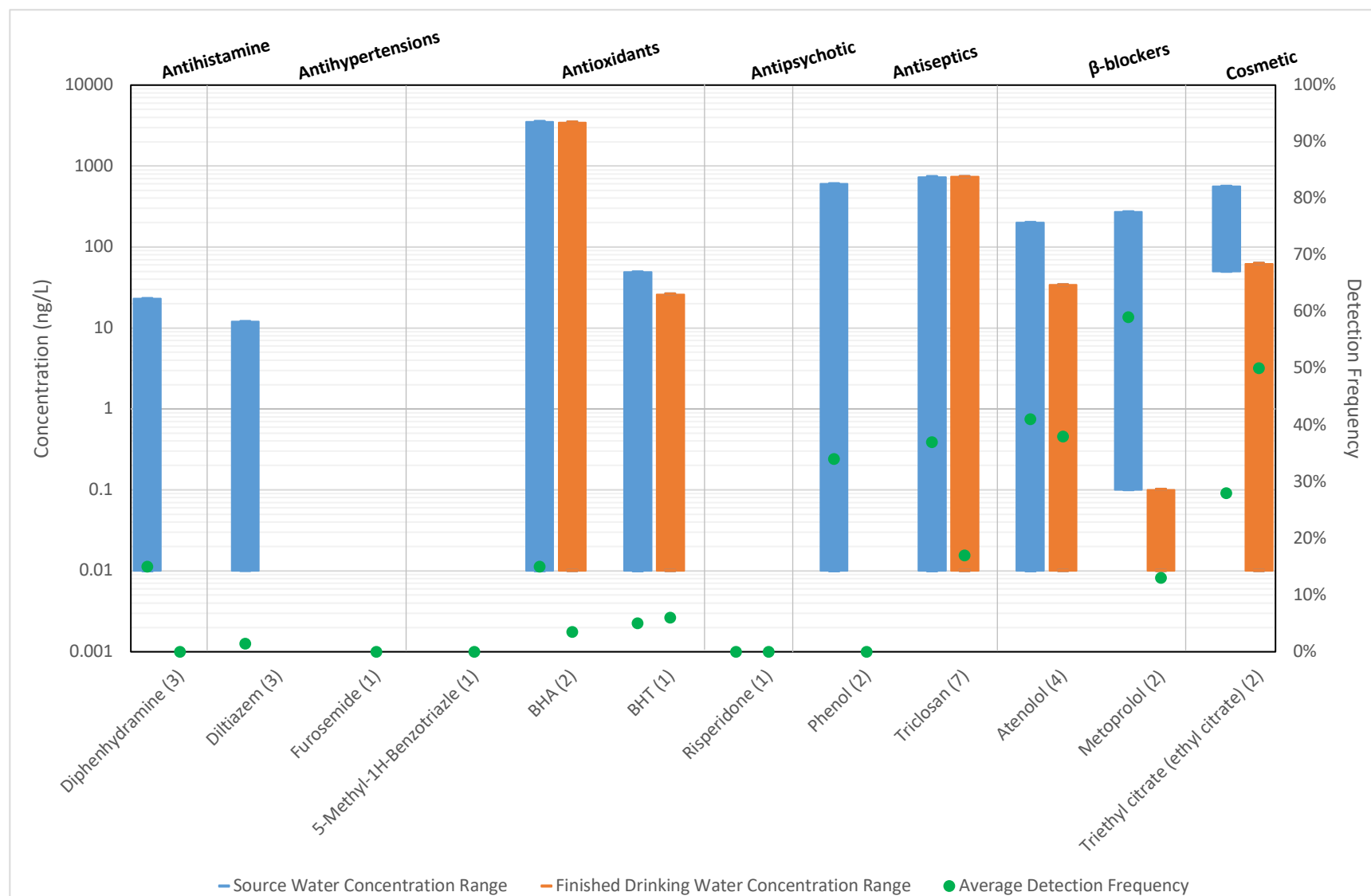


Figure S26. Concentration range of antihistamine, antihypertensions, antioxidants, antipsychotic, antiseptics, β -blockers, and cosmetic detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

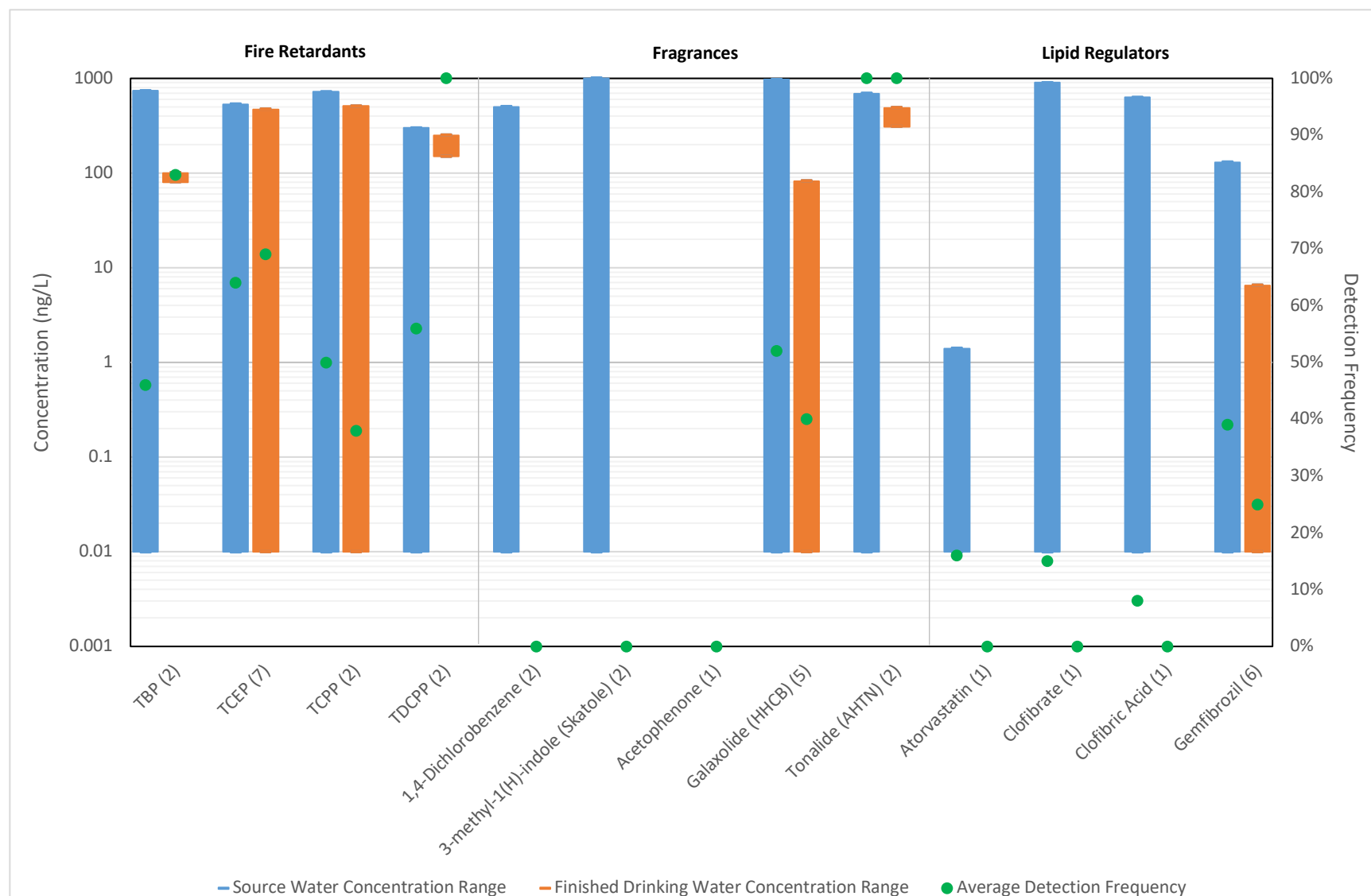


Figure S27. Concentration range of fire retardants, fragrances, and lipid regulators detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

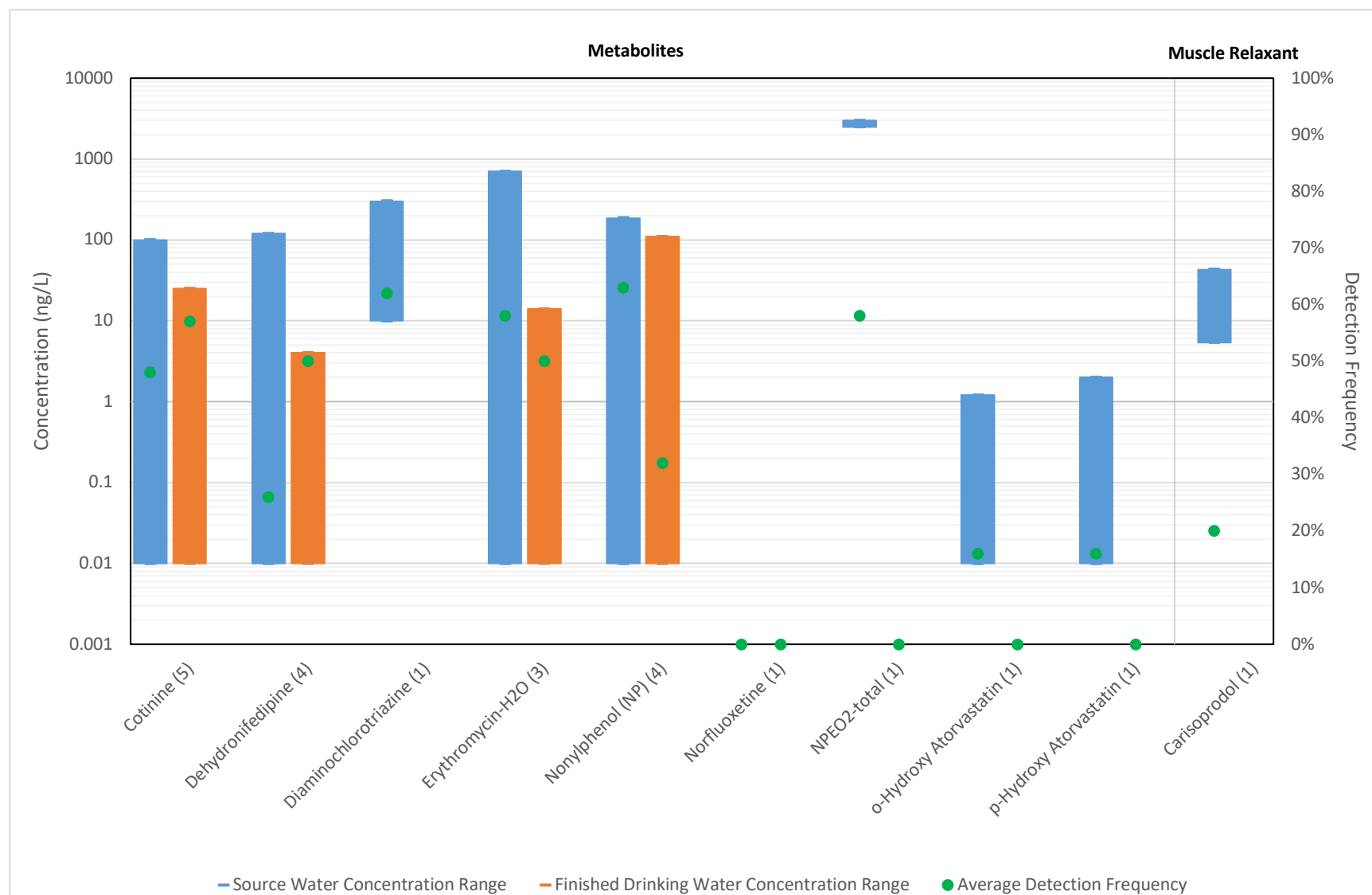


Figure S28. Concentration range of metabolites and muscle relaxant detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

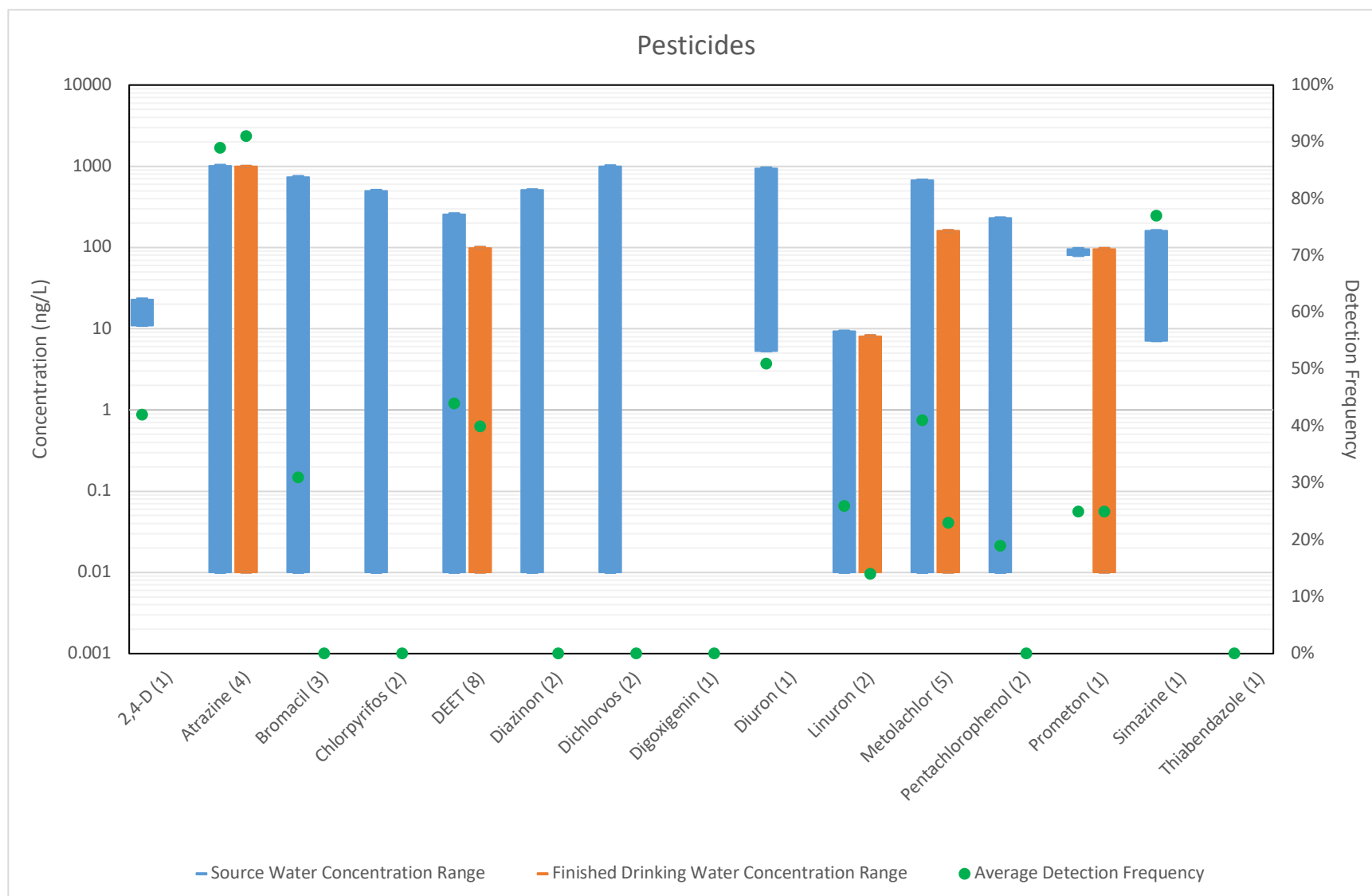


Figure S29. Concentration range of pesticides detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

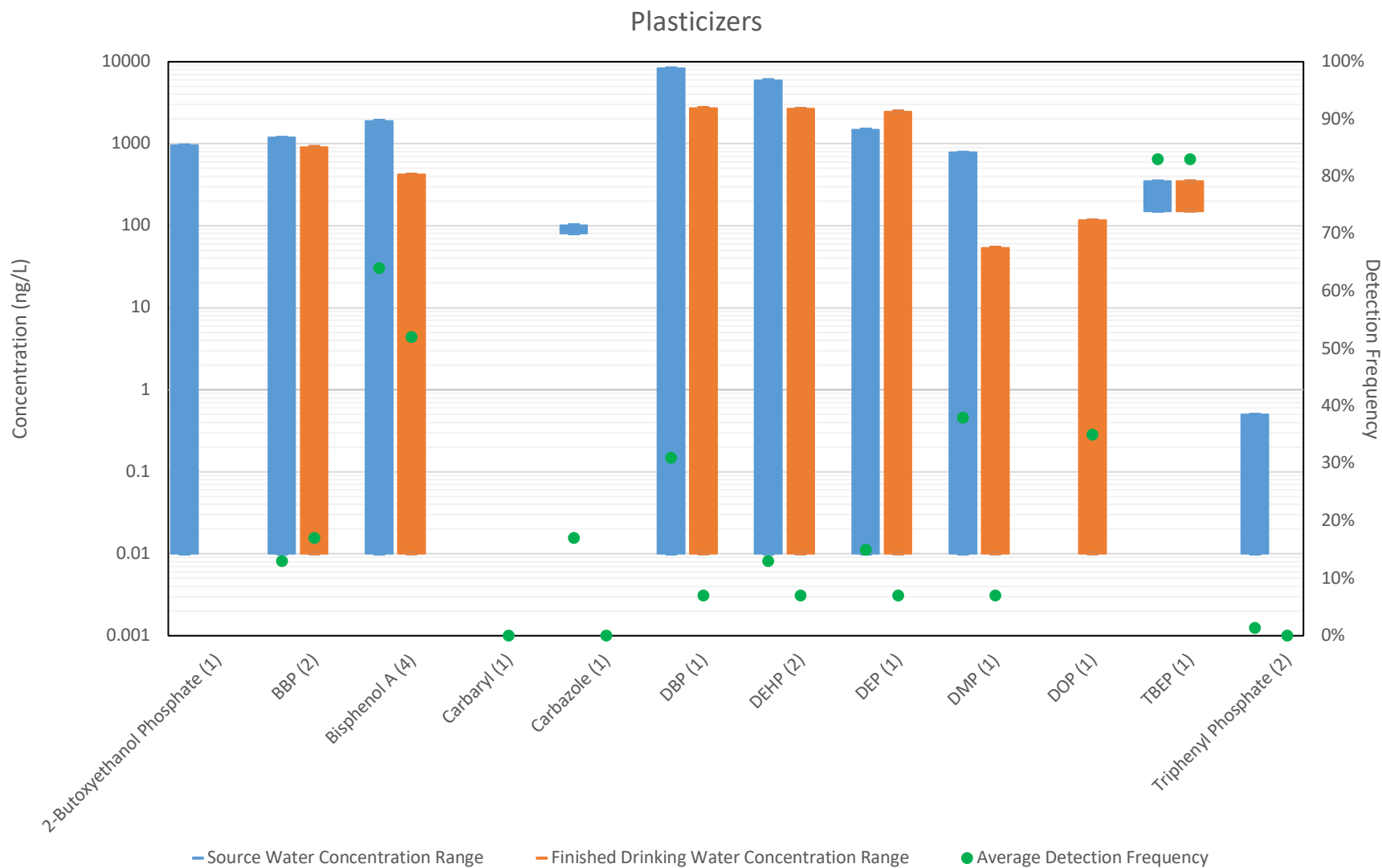


Figure S30. Concentration range of plasticizers detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

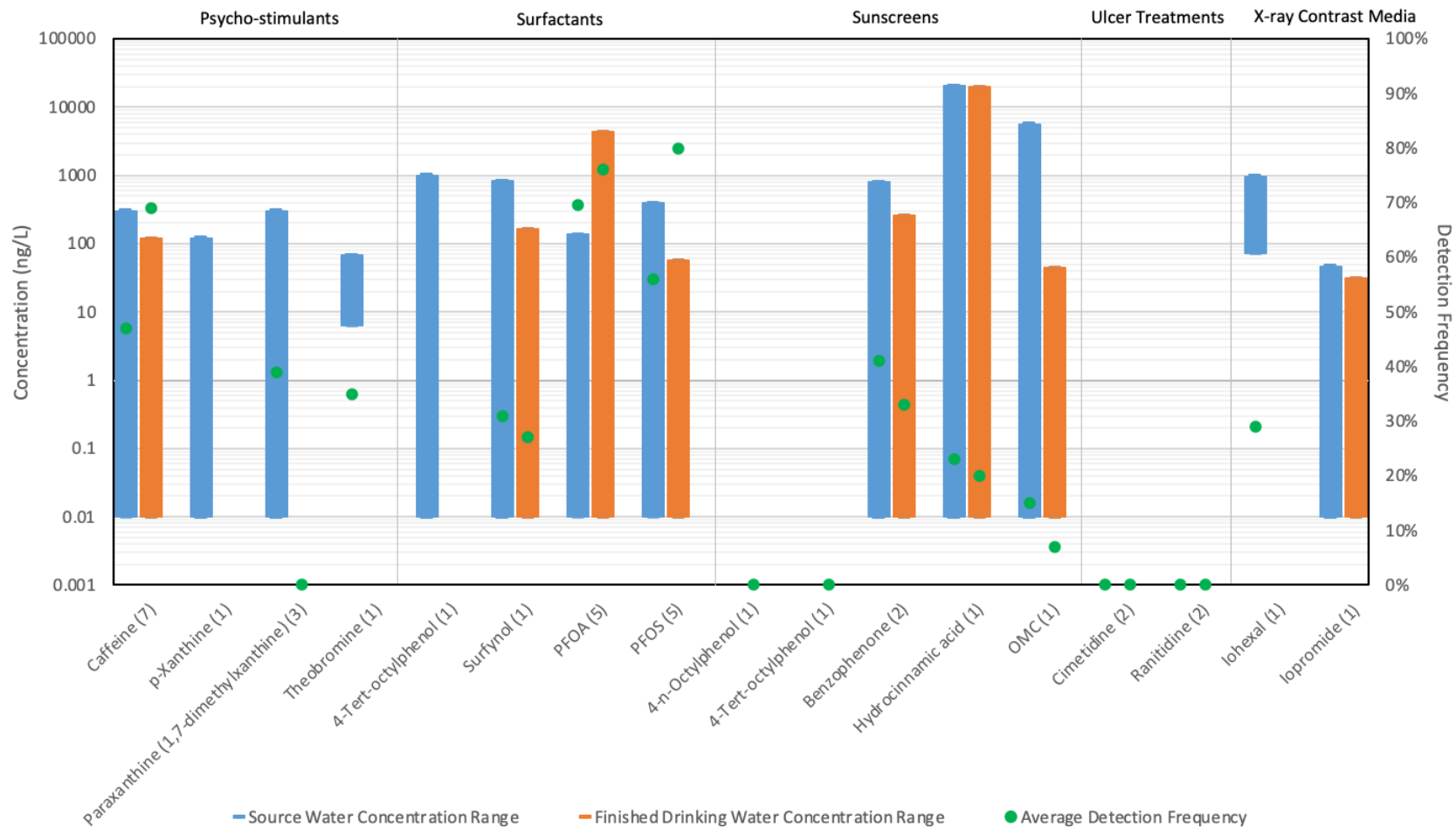


Figure S31. Concentration range of psycho stimulants, surfactants, sunscreens, ulcer treatments, and x-ray contrast media detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

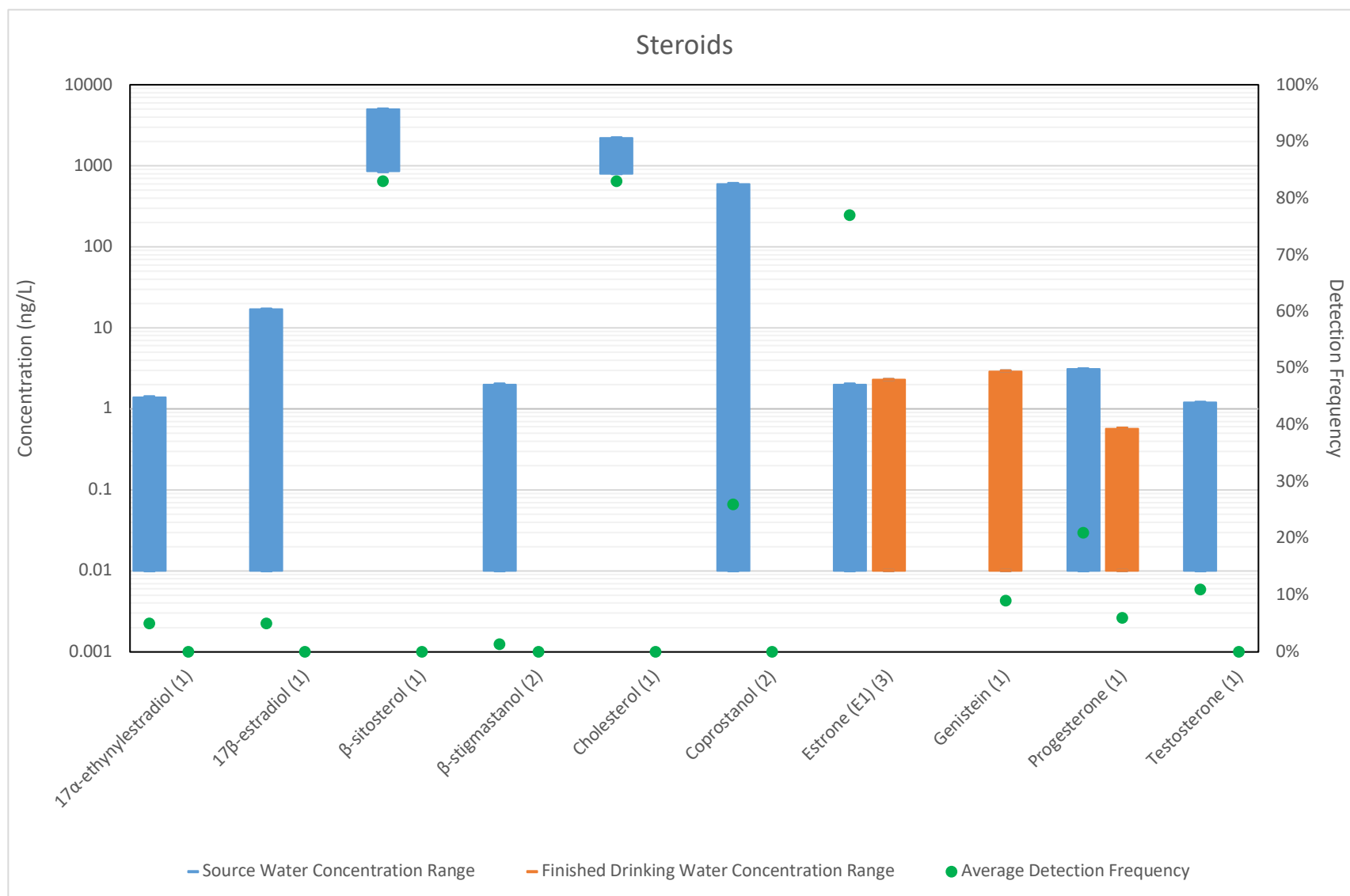


Figure S32. Concentration range of steroids detected in WTP source water (blue bar) and finished drinking water (orange bar) and their average detection frequency (green dots). Number of studies on the compounds is indicated in the parentheses (data from Table S7).

Table S1. Top Therapeutic Classes by Dispensed Prescriptions in the U.S. (IMS Institute for Healthcare Informatics, 2012)

Top Therapeutic Classes by U.S. Dispensed Prescriptions Total Rx in Millions						
RANK		2007	2008	2009	2010	2011
	Total US Prescription Market	3,825	3,866	3,949	3,993	4,024
1	Antidepressants	237	241	247	254	264
2	Lipid Regulators	233	242	254	260	260
3	Narcotic Analgesics	231	239	241	244	238
4	Antidiabetes	165	166	169	172	173
5	Ace Inhibitors (Plain & Combo)	159	163	166	168	164
6	Beta-Blockers (Plain & Combo)	162	164	163	162	161
7	Respiratory Agents	147	147	152	153	153
8	Anti-Ulcerants	134	139	146	147	150
9	Diuretics	137	135	132	131	128
10	Anti-Epileptics	102	110	116	122	128
11	Tranquillizers	98	101	104	108	111
12	Thyroid Preparations	103	104	105	107	110
13	Calcium Antagonists (Plain & Combo)	87	90	93	96	98
14	Antirheumatic Non-Steroid	90	91	92	93	97
15	Hormonal Contraceptives	94	94	93	91	90
16	Angiotensin II	83	86	85	84	86
17	Broad Spectrum Penicillins	77	74	77	76	77
18	Macrolides & Similar Type Antibiotics	63	66	69	67	69
19	Hypnotics & Sedatives	58	60	63	63	63
20	Vitamins and Minerals	60	59	58	58	60

Table S2. Top Therapeutic Classes by U.S. Sales (IMS Institute for Healthcare Informatics, 2012)

Top Therapeutic Classes by U.S. Sales US Dollar in Billions						
RANK		2007	2008	2009	2010	2011
	Total US Prescription Market	280.5	285.7	300.7	308.6	319.9
1	Oncologics	18.1	19.7	21.5	22.3	23.2
2	Respiratory Agents	15.1	16.0	18.1	19.3	21.0
3	Lipid Regulators	19.4	18.1	18.6	18.8	20.1
4	Antidiabetics	12.2	13.6	15.8	17.7	19.6
5	Antipsychotics	12.8	14.3	14.7	16.2	18.2
6	Autoimmune Diseases	7.6	8.6	9.7	10.6	12.0
7	Antidepressant	11.7	11.7	11.5	11.6	11.0
8	HIV Antivirals	6.2	7.1	8.2	9.3	10.3
9	Anti-Ulcerants	14.6	14.2	14.1	11.9	10.1
10	Narcotic Analgesics	6.7	7.3	8.0	8.4	8.3
11	ADHD	4.0	4.7	5.8	6.7	7.9
12	Platelet Aggregation Inhibitors	5.0	5.7	6.5	7.1	7.8
13	Angiotensin II	6.5	7.6	8.6	8.7	7.6
14	Multiple Sclerosis	3.4	4.1	5.0	5.8	7.1
15	Vaccines (Pure, Comb, Other)	5.9	5.0	4.7	5.7	6.3
16	Anti-Epileptics	10.0	11.1	6.9	5.6	5.9
17	Hormonal Contraceptives	4.1	4.5	4.7	4.8	5.2
18	Erythropoietins	8.4	6.9	6.3	6.1	5.1
19	Immunostimulating Agents	4.1	4.1	4.1	4.2	4.5
20	Antivirals, Excl. Anti-HIV	3.6	3.9	4.8	3.2	3.7

Table S3. Most commonly used active ingredients in conventional pesticides for the agricultural market sector, 1987 to 2007 estimates (ranked by range in millions of pounds of active ingredient) (adapted from Kiely et al., 2004; Grube et al., 2011)

Active Ingredient	Type	2007		2005		2003		2001		1999		1997		1987	
		Rank	Range	Rank	Range	Rank	Range	Rank	Range	Rank	Range	Rank	Range	Rank	Range
Glyphosate	H	1	180-185	1	155-160	1	128-133	1	85-90	2	67-73	5	34-38	17	6-8
Atrazine	H	2	73-78	2	70-75	2	75-80	2	74-80	1	74-80	1	75-82	1	71-76
Metam Sodium	Fum	3	50-55	3	39-44	3	45-50	3	57-62	3	60-64	3	53-58	15	5-8
Metolachlor-s	H	4	30-35	5	27-32	6	28-33	9	20-24	12	16-19	NA	NA	NA	NA
Acetochlor	H	5	28-33	6	26-31	5	30-35	4	30-35	4	30-35	7	31-36	NA	NA
Dichloropropene	Fum	6	27-32	4	30-35	7	20-24	8	20-25	11	17-20	6	32-37	4	30-35
2,4-D	H	7	25-29	7	24-28	4	30-35	5	28-33	6	28-33	8	29-33	5	29-33
Methyl Bromide	Fum	8	11-15	8	12-16	8	13-17	7	20-25	5	28-33	4	38-45	NA	NA
Chloropicrin	Fum	9	9-11	10	9-12	9	9-12	18	5-9	NA	NA	NA	NA	NA	NA
Pendimethalin	H	10	7-9	9	9-12	10	9-12	11	15-19	10	18-22	9	4-28	10	10-13
Ethephon	PGR	11	7-9	11	8-10	15	6-7	21	5-8	24	5-6	NA	NA	NA	NA
Chlorothalonil	F	12	7-9	13	7-9	14	7-9	13	8-11	13	8-11	15	7-10	19	5-7
Metam Potassium	Fum	13	7-9	20	4-6	20	4-6	NA	1-2	NA	NA	NA	NA	NA	NA
Chlorpyrifos	I	14	7-9	15	6-8	13	7-9	15	7-10	16	8-10	14	9-13	14	6-9
Copper Hydroxide	F	15	6-8	12	8-10	12	7-9	14	8-10	15	8-10	13	10-13	19	5-7
Simazine	H	16	5-7	17	5-7	17	6-7	23	5-7	NA	NA	NA	NA	NA	NA
Trifluralin	H	17	5-7	14	7-9	11	8-10	12	12-16	9	18-23	10	1-25	6	25-30
Propanil	H	18	4-6	18	4-6	18	5-7	17	6-9	18	7-10	22	6-8	13	7-10
Mancozeb	F	19	4-6	16	6-8	16	6-7	20	6-8	21	6-8	17	7-10	21	4-6
Aldicarb	I	20	3-4	21	3-5	25	4-6	NA	3-5	NA	NA	NA	NA	NA	NA
Acephate	I	21	2-4	24	2-4	NA	1-3	NA	1-3	NA	NA	NA	NA	NA	NA
Diuron	H	22	2-4	19	4-6	21	2-6	NA	3-6	NA	NA	NA	NA	NA	NA
MCPA	H	23	2-4	NA	2-4	24	4-6	NA	3-5	NA	NA	NA	NA	NA	NA
Paraquat	H	24	2-4	25	2-4	NA	3-4	NA	3-5	NA	NA	NA	NA	NA	NA
Dimethenamid	H	25	2-4	NA	2-4	23	4-6	19	6-8	20	6-8	20	6-9	NA	NA

H – Herbicide; I – Insecticide; F – Fungicide; Fum – Fumigant; PGR – Plant Growth Regulator; NA – an estimated is not available; 2,4-D – 2,4-Dichlorophenoxyacetic acid;

MCPA – 4-chloro-2-methylphenoxy acetic acid.

Table S4. Total excretion of the CECs reported in literature

Class	Compound	Total Excretion (%)^{[1],[2],[3]}
Analgesic	Acetaminophen	83
	Diclofenac	16-51
	Ibuprofen	5-100
Antibiotic	Sulfamethoxazole	20-98
	Trimethoprim	40-69
Antidepressant	Diazepam	85
	Fluoxetine	71
Antiepileptic	Carbamazepine	21-63
β -Blocker	Atenolol	69-96
	Metoprolol	11-93
	Propranolol	100
Lipid Regulator	Gemfibrozil	5-50

[1] Lienert et al., 2007; [2] Luo et al., 2014; [3] ter Laak, et al., 2010.

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Analgesics	Acetaminophen (Paracetamol)		960							[2]
			960				ND			[3]
								1060	50	[5]
						ND		260		[6]
			>2,000				130			[11]
							79	1,500	14	[12]
						<50				[15]
			61683		100		98		100	[16]
		370	41700	218000		ND	85.5	210		[17]
			39500				ND			[19]
	Aspirin Brompheniramine Codeine	170	440	930		ND	29.4	70		[17]
			40				ND			[11]
								730	72.5	[5]
	Diclofenac		15				3			[19]
			116				<0.5			[2]
			110				90			[3]
							165			[8]
		ND		14		8.3		177		[9]
	Hydrocodone Ibuprofen					<10		440		[13]
								<10		[15]
		86	277	580		ND	12	120		[17]
			36				35			[19]
							22	92	44	[12]
			1900				250			[3]
						5		425		[4]
						ND		88		[6]
	Indomethacin Mefenamic Acid Naproxen						13			[8]
							460	4200	46	[12]
						<10				[15]
		8600	22300	56500		13	55.8	92		[17]
			12053				ND			[19]
			54				11			[19]
			3				6			[19]
			22500				<1.0			[2]
			3200				380			[3]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued).

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Analgesics	Naproxen	9300	35700 13418 1200	210000		26		172		[4]
						81		106		[7]
							72			[8]
						<20		3680		[13]
						ND	30.3	150		[17]
	Ketoprofen	150	563 97	1300			5			[19]
							280			[3]
						ND		29		[4]
	Oxycodone					ND	29	65	60	[17]
						ND	ND			[19]
Antagonists	Propoxyphene					53		150	25	[6]
							53	310		[12]
						ND		65		[6]
Antisthmas	Salicylic Acid	434		8,036			17	34	0	[12]
								25		[9]
						ND		1680		[13]
						40		0.9		[6]
Antibiotics	Benztropine					ND		ND	54	[12]
							ND	ND		[6]
							110			[11]
							14	35		[12]
							9			[19]
	Theophylline		12						8	[12]
							<88	<88		[10]
							690			[19]
	Azithromycin	ND	1083	16	33.3	ND		ND	0	[9]
							ND			[16]
	Chlortetracycline	12	178	377		8.8		110	61	[9]
							67	260		[12]
	Ciprofloxacin							16		[15]
						<10				[19]
							67			[9]
	Clarithromycin	ND	2747	106		ND		611		[9]
							103			[19]
	Clindamycin	6.8	122	13		15		33		[9]
	Demeclocycline		ND		0		ND		0	[16]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Antibiotics	Doxycycline		738		100		370		33.3	[16]
	Erythromycin							ND	0	[5]
								610	52.5	[5]
						<10	2	15		[15]
			ND		0		ND		0	[16]
	Florfenicol						ND	ND	0	[12]
	Levofloxacin					<10		10		[15]
	Lincomycin						ND	ND	0	[12]
						<10				[15]
			58		83.3		35		66.7	[16]
	Metronidazole		169				229			[19]
	Ofloxacin						160	660	90	[12]
	Oxytetracycline		29		100		17		33.3	[16]
	Sulfachloropyridazine						2			[10]
	Sulfadiazine		37		33.3		28		16.7	[16]
			65				30			[19]
	Sulfadimethoxine	ND		2.6		ND		1.9		[9]
							67			[10]
							ND	ND	0	[12]
	Sulfamerazine		ND		0		ND		0	[16]
	Sulfamethazine	ND		27		ND		ND		[9]
							5			[10]
							12	87	2	[12]
			26		16.7		ND		0	[16]
			ND				26			[19]
	Sulfamethazole						1			[10]
	Sulfamethoxazole		2060				5			[2]
								763	72.5	[5]
						98		2200		[6]
							443			[8]
		14		261		79		472		[9]
							141			[10]
							330	2900	90	[12]
		846	1786	3905	100	ND	304	1328	89	[14]
						35	80	140		[15]
			1566		100		178		100	[16]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Antibiotics	Sulfamethoxazole		1216				570			[19]
	Sulfisoxazole	ND		22		ND		12		[9]
	(Sulfafurazole)									
	Tetracycline	ND		39		ND		31		[9]
						<10				[9]
			310		83.3		ND		0	[16]
			2512				111			[19]
	Trimethoprim		1140				<0.5			[2]
								414	60	[5]
						39		140		[6]
Anti-cancer							620			[8]
							90	370	86	[12]
						<10				[15]
	Tylosin		220				18			[19]
	Tamoxifen		ND		0		ND		0	[16]
Anticoagulants	Warfarin		11				2			[19]
						ND		50		[6]
Antidepressants	Amitriptyline						ND	ND	0	[12]
						25		86		[6]
			>2,000				1,490			[11]
							11	110	40	[12]
	Alprazolam					10		18		[6]
							10	31	30	[12]
		3.09	6.24	12.6	100	5.01	6.2	8.21	100	[20]
	Bupropion					<10		4300		[18]
		17.1	110	231	100	35.9	118	310	100	[20]
	Citalopram					<10		520		[18]
		77.7	133	170	100	205	280	414	100	[20]
	Diazepam		<2.5				3.7			[2]
							3			[8]
			40				40			[11]
	Fluoxetine	2.29	3.38	4.57	100	<0.05	1.62	3.5	71	[20]
			17				25			[2]
							44			[8]
							8.7	31	37.5	[12]
						<10		76		[18]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Antidepressants	Fluoxetine		144			40	27	73		[19]
	Lorazepam	9.14	7	33	100	37.3	3	85.5	100	[6] [19]
	Meprobamate		20.3				64.2			[20]
			1440				1270			[2]
	Oxazepam	2.3	8.43	16.9	100	7.09	603	14.4	100	[8]
	Paroxetine					2.5	9.87	13		[20]
							ND	ND	0	[6]
	Promethazine		270				16			[12] [19]
	Sertraline					0.4	ND	16	0	[6] [12]
						57	87			[6]
Antidiabetics	Venlafaxine	46.7	80.8	114	100	27.9	21	71	64	[12]
						<10	62.8	88.3	100	[20]
	Glibenclamide	169	415	609	100	389	480	553	100	[18] [20]
	Glipizide		12			ND	7			[19] [6]
Antiepileptics	Glyburide					ND		30		[6]
	Carbamazepine		232			ND		120		[6]
							187			[2]
						ND		59		[4]
						70		270	82.5	[5]
								800		[6]
		25		51			180			[8] [9]
			600			34		111		[10]
							120			[11]
							140			[12]
		66	137	348	100	66	97	240	96	[14]
						<10	156	270	100	[15]
			110		100			12		[16]
		34	115	350		ND	155	62	100	[17]
						<10	21.3	1500		[18]
			386				223			[19]
		61	145	347	100	150	310	731	100	[20]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Antiepileptics	Gabapentin		100			<10	ND	3100		[3]
	Lamotrigine					<10		1200		[18]
	Oxcarbazepine					<10		480		[18]
	Phenytoin (Dilantin)		402				287			[2]
			450				250			[3]
Antihistamine	Primidone						600			[8]
							183			[8]
			130				100			[11]
	Valproic Acid		140		25		46	120		[15]
	Diphenhydramine						ND		55	[3]
Antihypertensions								387		[5]
		286	462	615	100	<0.05	589		86	[10]
	Famotidine		635				194	704		[20]
	Loratadine		26				145			[19]
							6			[19]
Antihypertensions	Amlodipine						6.9	18	22	[12]
	Clonidine						ND	ND	0	[12]
	Clopidogrel	7.4	35.5	92.8	100	13.9	21.8	30.1	100	[20]
	Desmethyldiltiazem					65		110		[6]
							24	100	18	[12]
	Diltiazem							146	67.5	[5]
						28		200		[6]
		ND		69		ND		107		[9]
							85	340	84	[12]
		15.3	105	215	100	179	194	218	100	[20]
	Enalapril		35				0.85			[2]
							4.6	38	27	[12]
			83				ND			[19]
	Enalaprilat						14	150	10	[12]
	Furosemide				180			930		[6]
Antihypertensions							280	810	90	[12]
	Hydrochlorothiazide		1830				497			[19]
						1300		2950		[6]
							1100	2800	100	[12]
			2325				1453			[19]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Antihypertensions	Lisinopril		2693				180 ND	3300	47	[12] [19]
	Triamterene					130		440		[6]
	Valsartan					60	37	170	70	[12]
	Verapamil					14	1600	5300	98	[6] [12]
							26	190	80	[6]
Antineoplastics	5-Fluorouracil	5.34	18.5	42.8	100	28.8	49.2	63.2	100	[12] [20]
	Antioxidents		ND				ND			[3]
Antipsychotics	5-Methyl-1H-Benzotriazole							1700	45	[5]
	Aripiprazole	ND	5.58	22.4	57	ND	10.3	20.9	86	[20]
	Quetiapine	11	24.4	43.6	100	ND	0.98	3.43	57	[20]
Antiseptics	Risperidone		<2.5				<0.5			[2]
	4-Chloro-m-cresol		600				ND			[3]
	Biosol		250				ND			[3]
	Biphenylol		900				100			[3]
	Chlorophene		750				200			[3]
	Chloroxylenol (PCMX)		400				80			[3]
	Ciclopirox		1,410				321			[11]
	Terbinafine		510				120			[11]
	Triclosan		1280				<2.0			[2]
						10		1600	62.5	[5]
Barbiturates								21		[7]
							203			[8]
						<10				[10]
		180	2300	4400		ND	48.4	160		[17]
			800				250			[3]
	Butalbital		62				50			[19]
	Pentobarbital		92				67			[19]
	Phenobarbital		70				ND			[3]
			101				118			[19]
	Secobarbital		ND				ND			[3]
β-blockers	Atenolol		3060				879			[2]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
β-blockers	Atenolol	377		2000	100	120		960		[6]
	Metoprolol					1267		[8]		
						940	3,000	96	[12]	
						208		[19]		
						382	754	100	[20]	
						ND	1,200	88	[1]	
						150	650		[6]	
	Nadolol					130			[11]	
						410	660	98	[12]	
						1518	908		[19]	
						52	360	71	[1]	
						ND			[19]	
			Propranolol				26	1,900	100	[1]
						32	77		[6]	
						33	260	88	[12]	
						62			[19]	
						82.2	225	100	[20]	
						246			[19]	
Cosmetics	Sotalol	3.04		53.8	100					[19]
	Triethyl citrate (ethyl citrate)						520	72.5	[5]	
Fire Retardants	TBP						470	70	[5]	
	TCEP						480	75	[5]	
	TCPP					543				[8]
						480	77.5	[5]		
						3750				[8]
								910	27.5	[5]
Fragrances	1,4-Dichlorobenzene	240	1376	4020	100	145		530	57.5	[5]
	Galaxolide (HHCB)							1104	100	[14]
Lipid Regulators	Musk Ketone						465			[8]
	Tonalide (AHTN)						48	2600	80	[5]
	Atorvastatin		201				<0.5			[2]
						ND		42		[6]
							58			[8]
						<38	<38	<38	8	[12]
			939				ND			[19]
	Bezafibrate		4				ND			[19]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Lipid Regulators	Fenofibrate		250				ND			[11]
			317				3			[19]
	Gemfibrozil		4770				9.0			[2]
			410				130			[3]
						ND		158		[4]
						47		1220		[6]
							890			[8]
		182		451		ND		42		[9]
							420	2300	76	[12]
						63		3830		[13]
		315	934	1757	100	6	41	207	100	[14]
		1090	467	8500		ND	151	650		[17]
			1220				42			[19]
	Mevastatin		507				ND			[19]
	Pravastatin		783				ND			[19]
	Simvastatin		<2.5				<0.5			[2]
Metabolites							<41	<41	24	[12]
	Simvastatin Hydroxy Acid		10				<0.5			[2]
	10-OH-CBZ					<10		1900		[18]
	2-Diphenhydramine acetic acid	<0.05	3.7	5.52	86	<0.05	4.5	12.9	29	[20]
	2-Hydroxy-Ibuprofen					ND		200		[6]
	4-Nonylphenol							38000	62.5	[5]
	Diethoxylate									
	4-Nonylphenol							18000	62.5	[5]
	Monoethoxylate									
	4-Octylphenol							360	32.5	[5]
	Diethoxylate									
	10-Hydroxy-Amitriptyline					ND		64		[6]
						<5	<5	<5	12	[12]
	α -Hydroxy Alprazolam	5.86	21.4	28.5	100	7.25	9.2	12.4	100	[20]
	Clopidogrel	43.5	160	278	100	166	194	249	100	[20]
	Carboxylic Acid									

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Metabolites	Cotinine	41		1,581		ND		1030 ND	92.5	[5] [9] [10]
		130		2,700			147			[21]
	Dehydroaripiprazole	ND	ND	ND	0	ND	ND	ND	0	[20]
	Dehydronifedipine							22	57.5	[5]
	Desacetyl Diltiazem	125	483	1090	100	163	294	368	100	[20]
	Desmethylsertraline (Norsertaline)						9.9	24	18	[12]
		23.7	71.1	137	100	ND	54.4	78.6	86	[20]
	DMV					<10		10000		[18]
	DiOH-CBZ					<10		400		[18]
	Glu-LMG					<100		455		[18]
	Hydroxybupropion					<10		2000		[18]
	N-desmethylocitalopram					<10		200		[18]
		ND	55.4	126	71	35.9	118	310	100	[20]
	Nonylphenol (NP)		130				103			[11]
						<50		3610		[13]
		220	510	870		ND	9	50		[17]
	Nordiazepam	1.68	5.3	9.73	100	3.05	4.53	6.56	100	[20]
	Norfluoxetine		9.9				3.9			[2]
						1.2		1.2		[6]
							7.7	15	17	[12]
	Norquetiapine	39.5	71	159	100	25	74.3	131	100	[20]
	Norverapamil					42		71		[6]
		4.2	14.8	33.5	100	2.6	5.8	20	52	[12]
	NPEC		5465				20.3	39.9	100	[20]
	<i>o</i> -Hydroxy Atorvastatin		196				25159 <1.0			[19] [2]
	<i>p</i> -Hydroxy Atorvastatin		280				<1.0			[2]
	PEG		39237				1606			[9]
	<i>Threo/erythro</i> - hydrobupropion					<10		5700		[18]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Muscle Relaxants Pesticides	Carisoprodol		410				141			[11]
	Atrazine		<2.5				0.81			[2]
							3			[8]
	DEET							2100	70	[5]
							106			[8]
			450				774			[10]
							120			[11]
						<10	18	30		[15]
	Diazinon							150	47.5	[5]
	Linuron		<5.0				0.73			[2]
Plasticizers	Metolachlor							97	37.5	[5]
	Pentachlorophenol							86	35	[5]
	Phenol							1800	40	[5]
	Thiabendazole						33			[10]
	2-Butoxyethanol							12000	70	[5]
	Phosphate									
	Bisphenol A (BPA)		320				<2.0			[2]
							43			[8]
						<10		697		[13]
		60	296	600		ND	12.6	81		[17]
Psycho-stimulants	<i>n</i> -Butylbenzene-sulfonamide		694				120			[11]
	Triphenyl Phosphate							180	37.5	[5]
	Amphetamine					0.2		0.2		[6]
							3.5	40	10	[12]
	Caffeine							7990	70	[5]
							43			[8]
		2,449		4,866		3.9		23.1		[9]
			>2,000				535			[10]
							60			[11]
			41204			<10	17	50		[15]
							76		100	[16]
		11500		120000	100					[21]
	Methamphetamine						350			[10]
	Paraxanthine (1,7-dimethylxanthine)							8550	35	[5]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq. %	WWTP Effluent (ng/L)			Freq. %	Ref.
		Minimum	Mean	Maximum		Minimum	Mean	Maximum		
Psycho-stimulants	Paraxanthine (1,7-dimethylxanthine)						112			[10]
Steroids	Ethinylestradiol (EE2)					<10				[15]
	Cholesterol							<10		[8]
	Coprostanol							8700	90	[5]
	Estradiol							5900	60	[5]
	Estone							3		[8]
								69		[8]
		ND	97	160		ND	3	30		[17]
	Fluocinonide						ND	ND	0	[12]
	Fluticasone						ND	ND	0	[12]
	Hydrocortisone						ND	ND	0	[12]
	Melengestrol Acetate						ND	ND	0	[12]
	Methylprednisolone						ND	ND	0	[12]
	Norethindrone						ND	ND	0	[12]
	Prednisolone						ND	ND	0	[12]
	Prednisone						ND	ND	0	[12]
	Progesterone							<0.5		[8]
						ND	<188	<188	4	[12]
	Sitosterol							2900	72.5	[5]
	Testosterone							<0.5		[8]
Surfactants							ND	ND	0	[12]
	4- <i>n</i> -Octylphenol		100				ND			[11]
	4- <i>Tert</i> -octylphenol					10		1860		[13]
		80	1340	3900		ND	48.4	100		[17]
	AEO		31213				167			[19]
	NPEO		24,363				314			[19]
	PFOA					14.8		65.2	100	[22]
		2		184		6.7		183		[23]
	PFOS					ND		47.7	95	[22]
		2.5		16		1.8		28		[23]
Ulcer Treatments	Allopurinol		10				ND			[11]
	Cimetidine					ND		410		[6]
			463				118			[19]
	Ranitidine					ND		550		[6]
							120	1400	38	[12]

Table S5. Occurrence of CECs that have been reported in WWTP influent and effluent in the United States (continued)

Groups	Compounds	WWTP Influent (ng/L)			Freq.	WWTP Effluent (ng/L)			Freq.	Ref.
		Minimum	Mean	Maximum	%	Minimum	Mean	Maximum	%	
Ulcer Treatments	Ranitidine		301				30			[19]
X-ray Contrast Media	Iopromide						<10			[8]

ND – not detected; Det – detected (concentration not specified); DEET – N,N-Diethyl-meta-toluamide; TCEP – tris-(2-chloroethyl)-phosphate; TCPP – tris-(2-chloroisopropyl)-phosphate; TBP – tributyl phosphate; DiOH-CBZ – 10,11-dihydro-10,11-dihydroxy-carbamazepine; 10-OH-CBZ – 10,11-dihydro-10-hydroxy-carbamazepine; Gluc-LMG – 2-N-glucuronide-lamotrigine; DMV – *O*-desmethyl-vorenlafaxine; PFOA – perfluorooctanoic acid; PFOS – perfluorooctanesulfonic acid.

AHAN – Acetyl-hexamethyl-tetrahydro-naphthalene; DBP – Dibutyl phthalate; DEHP – Di-(2-ethylhexyl) phthalate; NPEO – Nonylphenol Ethoxylate; AEO – Alcohol Ethoxylate; NPEC – Nonylphenol Polyethoxy Carboxylate; PEG – Polyethylene Glycol

[1] Huggett et al., 2003; [2] Vanderford and Snyder, 2006; [3] Yu et al., 2006; [4] Gross et al., 2004; [5] Glassmeyer et al., 2005; [6] Batt et al., 2008; [7] Boyd et al., 2003; [8] Gerrity et al., 2011; [9] Spongberg and Witter, 2008; [10] Bartelt-Hunt et al., 2009; [11] Bisceglia et al., 2010; [12] Kostich et al., 2014; [13] Bulloch et al., 2015; [14] Kwon and Rodriguez, 2014; [15] Yang et al., 2011; [16] Gao et al., 2012; [17] Yu et al., 2013; [18] Writer et al., 2013; [19] Lara-Martín et al., 2014; [20] Subedi and Kannan, 2015; [21] Chiaia et al., 2008; [22] Elmoznino et al., 2018; [23] Loganathan, et al., 2007.

Table S6. Occurrence of CECs that have been reported in surface water in the United States

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Analgesics	Acetaminophen (Paracetamol)	ND	8	10000	23.8%	[3]
		ND		63		[6]
		ND		19	13%	[9]
		<2.5		73	24%	[10]
				25.8		[12]
				111.3		[14]
	Codeine	ND		1000	10.6%	[3]
		<3.6		15	29%	[10]
	Diclofenac	ND		24	50%	[9]
		18		124		[12], [13]
	Hydrocodone			16.7		[14]
		ND		1000	9.5%	[3]
	Ibuprofen	2		42	50%	[4]
						[8]
		ND		133	38%	[9]
		<25		40.5		[12], [13]
				43.6		[14]
	Indomethacin	ND		ND	0%	[4]
	Ketoprofen	0.4		0.8	9%	[4]
	Naproxen	<5		200		[1]
		1		14	18%	[4]
		ND		9	13%	[9]
		<1		31	24%	[10]
	Oxycodone			93.1		[14]
	Propoxyphene			6.4		[14]
Antagonists	Benzotropine			3.7		[14]
Antiasthmas	Albuterol (Salbutamol)	ND		ND	0%	[3]
		<1.4		5.9	5%	[10]
				9.8		[14]
Antibiotics	Azithromycin	ND		670		[6]
		<3.7		22	24%	[10]
	Carbadox	<3.4		49	41%	[10]
		ND		ND	0%	[3]
	Chlortetracycline	ND		690	2.4%	[3]
	Ciprofloxacin	ND		30	2.6%	[3]

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Antibiotics	Ciprofloxacin	8		8	5%	[4]
	Clarithromycin	0.2		2	100%	[9]
	Doxycycline	ND		ND	0%	[3]
	Enrofloxacin	ND		ND	0%	[3]
	Erythromycin	3		34	18%	[4]
		0.3		3	100%	[9]
	Lavofloxacin	ND		1	38%	[9]
	Lincomycin	ND		120	1%	[3]
		0.1		1.8	36%	[4]
	Monensin	ND		35		[2]
	Narasin	ND		38		[2]
	Ofloxacin	<2.5		21	2%	[10]
	Oxacillin	<2.5		17	2%	[10]
	Oxytetracycline	ND		340	1.2%	[3]
	Roxithromycin	<4.3		39	21%	[10]
		0.3		1.7	9%	[4]
		ND		180	4.8%	[3]
	Salinomycin	ND		6		[2]
	Sarafloxacin	ND		ND	0%	[3]
	Sulfachloropyridazine	ND		ND	0%	[3]
	Sulfadimethoxine	ND		60	1.2%	[3]
		ND		3,956		[6]
	Sulfamerazine	ND		ND	0%	[3]
	Sulfamethazine	0.1		1.1	23%	[4]
		ND		472		[6]
	Sulfamethoxazole	ND		19000	12.5%	[3]
		0.2		2	41%	[4]
		ND		343		[6]
		ND		7	88%	[9]
		<4.1		77	83%	[10]
				932		[12]
				576.4		[14]
	Sulfanilamide	<2.9		20	5%	[10]
	Sulfathiazole	ND		ND	0%	[3]
		ND		7		[6]
	Tetracycline	ND		110	1.2%	[3]

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Antibiotics	Tetracycline Trimethoprim	ND	6.7	ND	0%	[4]
		ND		710	12.5%	[3]
		0.3		1	9%	[4]
						[8]
		2		11	100%	[9]
		<3.4		52	26%	[10]
				180		[12]
				60.9		[14]
Anticoagulants	Tylosin	ND		280	13.5%	[3]
		2		40	23%	[4]
		ND		ND	0%	[3]
		ND		ND	0%	[3]
Antidepressants	Virginiaamycin Warfarin			131.3		[14]
				25		[14]
				0.8		[14]
				6.1		[12]
		ND		12	1.2%	[3]
		ND		1	38%	[9]
		<3.5		62	10%	[10]
				24.8		[14]
				8.3		[14]
				1.5		[14]
Antidiabetics	Sertraline			19		[14]
		ND		150	4.8%	[3]
		<0.5		9200	100%	[10]
Antiepileptics	Carbamazepine	0.1		2	86%	[4]
		14		116		[5]
		ND		296		[6]
		1		4	100%	[9]
		<2.7		38	21%	[10]
		203		330		[12], [13]
				249.3		[14]
				291		[12]
		5		37		[5]
		8		1,412		[6]
Antihistamines	Diphenhydramine	<3.6		43	33%	[10]

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Antihypertensions	Desmethyldiltiazem			16.8		[14]
	Diltiazem	ND		49	13.1%	[3]
		<3.5		21	29%	[10]
				56.8		[14]
	Enalapril			1.9		[14]
	Enalaprilat	ND		ND	0%	[3]
	Furosemide			37.2		[14]
	Hydrochlorothiazide			619.9		[14]
	Triamterene			23.6		[14]
Antioxidants	Valsartan			319.4		[14]
	Verapamil			35.8		[14]
	2,6-di-tert-butylphenol	ND		110	3.5%	[3]
	2,6-di-tert-butyl-1,4-benzoquinone	ND		460	9.4%	[3]
	5-Methyl-1H-Benzotriazole	ND		2400	31.5%	[3]
	BHA	ND		200	2.4%	[3]
	BHT	ND		100	2.4%	[3]
	Phenol	ND		1300	8.2%	[3]
	Triclocarban			102		[12]
Antiseptics		<0.5		9.9	12%	[10]
	Triclosan	ND		2300	57.6%	[3]
		ND		9.2	21%	[7]
		ND		106	63%	[9]
		<0.5		41	71%	[10]
		10.7		26.3		[12], [13]
	Atenolol	ND		ND	0%	[9]
				186.4		[14]
	Metoprolol	0.1		0.3	100%	[9]
Cardiac Stimulant Fire Retardants			0.7	217.7		[14]
	Propranolol					[8]
				11.2		[14]
	Digoxin	ND		ND	0%	[3]
	BDE 47			2.2		[12]
	BDE 99			0.9		[12]
	TCEP	ND		540	57.6%	[3]

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Fire Retardants	TCEP	ND	19.3	53	88%	[8]
				785		[9]
				2900		[12]
				160		[12]
Fragrances	TCPP TDCPP	ND		1345	12.9%	[3]
				4300		[12]
				410		[3]
				794		[3]
				2753		[11]
				112		[12], [13]
Lipid Regulators	Tonalide (AHTN)	56		188		[11]
				4		[12]
	Bezafibrate	0.5		100	32%	[4]
				12		[1]
	Clofibric Acid	2		790	14%	[4]
				4		[3]
	Gemfibrozil	ND		4	3.6%	[4]
				43		[64%]
				324		[10]
				112.5		[13]
Metabolites	10-Hydroxy-Amitriptyline	ND		900	38.1	[14]
				210		[3]
	Cotinine	3		3	25%	[6]
				21		[9]
	Dehydronifedipine	ND		30	19%	[10]
				7		[3]
	Desmethylertraline (norsertaline)	ND		1700	14.3%	[14]
				186		[3]
	Digoxigenin	ND		0%		[9]
				21.5%		[14]
	Erythromycin-H ₂ O	53		100%		[3]
				15.4		[9]
	Nonylphenol (NP)	ND		30.4		[14]
				75		[14]
Pesticides	Norfluoxetine	3		100%		[9]
				17.1		[12]

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Pesticides	Bifenthrin			3.6		[12]
	Carbaryl	ND		100	16.5%	[3]
	cis-Chlordane	ND		100	4.7%	[3]
	Chlorpyrifos	ND		310	15.3%	[3]
				4.9		[12]
	Diazinon	ND		350	25.9%	[3]
	Dieldrin	ND		210	4.7%	[3]
	DEET	ND		1100	74.1%	[3]
		7		1,617		[6]
		ND		68	66%	[7]
		2.3		3.3		[8]
		23		256	100%	[9]
				860		[12]
	Fipronil	22.2		28.7		[12], [13]
	Fipronil Desulfinyl			13.8		[12]
	Fipronil Sulfide			2		[12]
	Fipronil Sulfone			10.6		[12]
	Lindane	ND		110	5.9%	[3]
	Mecoprop	7.9		12.3		[8]
	Methyl Parathion	ND		10	1.2%	[3]
Plasticizers	Permethrin	<0.17		1.7		[12], [13]
	Thiabendazole	ND		27		[6]
	2-Butoxyethanol	ND		6700	45.9%	[3]
	Phosphate					
	Bisphenol A	ND		12000	41.2%	[3]
		1		1967	50%	[4]
		ND		190	44%	[7]
		ND		22	75%	[9]
		<1		691		[12], [13]
	DEHA	ND		10000	3.5%	[3]
Psycho-stimulants	DEHP	ND		20000	10.6%	[3]
	DEP	ND		420	11.1%	[3]
	Triphenyl Phosphate	ND		220	14.1%	[3]
	Amphetamine			7.1		[14]
	Caffeine	ND		6000	61.9%	[3]
		86		687		[5]

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.	
		Minimum	Mean	Maximum	%		
Psycho-stimulants	Caffeine	16		980		[6]	
		ND		68	85%	[7]	
		5		6.2		[8]	
		ND		16	50%	[9]	
		21		230	98%	[10]	
		Methamphetamine	ND		63		[6]
		Paraxanthine (1,7-dimethylxanthine)	ND		3100	28.6%	[3]
Steroids	17 α -Ethinylestradiol (EE2)	2		180		[6]	
		<11.6		57	45%	[10]	
		ND		831	15.7%	[3]	
	17 β -Estradiol	ND		200	10.6%	[3]	
		ND		1.8	21%	[7]	
	4-androstene-3,17-dione	<1.25		<5		[12], [13]	
		<0.5		17	31%	[10]	
	Cholesterol	ND		60000	84.3%	[3]	
		<150		2,896	96%	[7]	
	cis-androsterone	ND		214	14.3%	[3]	
	Coprostanol	ND		150000	85.7%	[3]	
		ND		67	44%	[7]	
	Coprostanone	ND		9.1	12%	[7]	
	Equilenin	ND		278	2.8%	[3]	
	Equilin	ND		147	1.4%	[3]	
		ND		5.5	18%	[7]	
	Estrone (E1)	ND		112	7.1%	[3]	
		1		1	9%	[4]	
		<10		200		[1]	
		ND		5.2	81%	[7]	
		<2.5		<5		[12], [13]	
				16.2		[14]	
	Fluticasone			16.2		[14]	
	Mestranol	ND		407	10%	[3]	
	Norethindrone	ND		872	12.8%	[3]	
	Progesterone	ND		199	4.3%	[3]	
		<0.7		88	15%	[10]	
				440.8		[14]	

Table S6. Occurrence of CECs that have been reported in surface water in the United States (continued)

Groups	Compounds	Surface Water (ng/L)			Detection Frequency	Ref.
		Minimum	Mean	Maximum	%	
Steroids	Stigmastanol	ND		4000	5.6%	[3]
	Testosterone	ND		214	2.8%	[3]
		<1.1		38	15%	[10]
Surfactants	PFOA		23.3	361.4		[14]
		ND		65.5	95%	[15]
		0.9		1.8		[16]
		2.6×10 ⁶		1.28×10 ⁹		[17]
				210,000	88%	[18]
		ND		100	92%	[19]
		5.1		830		[20]
		10		173		[21]
		<0.05		173		[22]
		0.27		47	100%	[23]
	PFOS	ND	7.6	11,000		[24]
		ND		27.7	31.3%	[15]
		1.8		2.1		[16]
		2×10 ⁵		3.68×10 ⁸		[17]
				8,970,000	96%	[18]
		ND		43	33%	[19]
		<5		7.4		[20]
		0.8		1,090		[21]
		<0.23		2,930		[22]
		ND		23	95%	[23]
		<0.25		1,090		[24]
Ulcer Treatments	Cimetidine	ND		580	9.5%	[3]
	Ranitidine	ND		10	1.2%	[3]
		<0.9		27	3%	[10]
				21		[14]

BHA – Butylated hydroxyanisole; BHT – Butylated hydroxytoluene; DBP – Dibutyl phthalate; DEHA – Di-(2-ethylhexyl) adipate; DEHP – Di-(2-ethylhexyl) phthalate; DEP – Diethyl phthalate; TCEP – tri(2-chloroethyl) phosphate; BDE 47 – Polybrominated diphenyl ethers-47; BDE 99 – Polybrominated diphenyl ethers 99; TCPP – tris-(2-chloroisopropyl)-phosphate; TDCPP – Tris(dichloroisopropyl) phosphate; PFOA – perfluorooctanoic acid; PFOS – perfluorooctanesulfonic acid.

[1] Boyd and Grimm, 2001; [2] Kim and Carlson, 2006; [3] Kolpin et al., 2002; [4] Tabe et al., 2009; [5] Guo and Krasner, 2009; [6] Bartelt-Hunt et al., 2009; [7] Singh et al., 2010; [8] Dougherty et al., 2010; [9] Padhye et al., 2014; [10] Blair et al., 2013; [11] Chase et al., 2012; [12] Sengupta et al., 2014; [13] Maruya et al., 2016; [14] Batt et al., 2016; [15] Bai and Son, 2021; [16] Goodrow et al., 2020; [17] Konwick et al., 2008; [18] Anderson et al., 2016; [19] Post et al., 2013; [20] Procopio et al., 2017; [21] Sinclair et al., 2006; [22] Vedagiri et al., 2018; [23] Zhang et al., 2016; [24] Crone et al., 2019.

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Analgesics	Acetaminophen (Paracetamol)	8	40	50%	ND	ND	0%	[1]
		ND	1890					[3]
		ND	160	8.1%				[5]
		ND	19.2	13%	ND	ND	0%	[8]
	Diclofenac	<1	9.5		<1	<1		[10]
		ND	1.2	21%	ND	ND	0%	[7]
		ND	24	50%	ND	9	25%	[8]
		7	10		ND	ND	0%	[1]
	Ibuprofen	ND	214					[3]
		ND	<240	2.7%				[5]
					ND	ND	0%	[1]
		ND	5,850	8%	ND	1,350	13%	[2]
	Naproxen	ND	270					[5]
		ND	132.9	38%	ND	10	13%	[8]
		<1	24		<1	32		[10]
			44	70%				[4]
		ND	32	58%	ND	ND	0%	[7]
		ND	9.2	13%	ND	5	13%	[8]
Antiasthmas	Albuterol (Salbutamol)	<1	11		<1	8		[10]
					ND	ND	0%	[1]
		ND	ND					[3]
Antibiotics	Amoxicillin	ND	ND	0%				[5]
		25	2200	23%				[9]
		ND	29	1.4%				[5]
	Azithromycin				ND	ND	0%	[1]
		ND	ND	0%				[5]
					ND	ND	0%	[1]
	Chlortetracycline	ND	ND	0%				[5]
					ND	ND	0%	[1]
								[5]
	Ciprofloxacin	ND	30	1.4%				[5]
		ND	1.7	100%	ND	0.2	75%	[8]
	Demeclocycline	0.2			ND	ND	0%	[1]
		ND	ND	0%				[5]
					ND	ND	0%	[1]
	Doxycycline	ND	ND	0%				[5]
		ND	ND	0%				[5]

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Antibiotics	Enrofloxacin	ND	40	6.8%	ND	ND	0%	[1]
	Erythromycin	<1	3.5		<1	1.5		[5]
	Levofloxacin	ND	1.3	38%	ND	ND	0%	[10]
	Lincomycin	ND	ND		ND	ND	0%	[8]
	Methotrexate	ND	ND	0%	ND	ND	0%	[1]
	Minocycline	ND	ND	0%	ND	ND	0%	[5]
	Norfloxacin	ND	ND	0%	ND	ND	0%	[1]
	Oxytetracycline	ND	ND	0%	ND	ND	0%	[5]
	Roxarsone	ND	ND	0%	ND	ND	0%	[1]
	Roxithromycin	ND	ND	0%	ND	ND	0%	[1]
	Sarafloxacin	ND	20	0%	ND	ND	0%	[5]
	Sulfadimethoxine	ND	ND	1.4%	ND	ND	0%	[1]
	Sulfamerazine	ND	ND	0%	ND	ND	0%	[5]
	Sulfamethazine	ND	ND	0%	ND	ND	0%	[1]
	Sulfamethizole	ND	ND	0%	ND	ND	0%	[5]
	Sulfamethoxazole	ND	ND	0%	ND	ND	0%	[1]
		4	10	17%				[3]
		ND	170					[4]
			173	91%		3	13%	[7]
		ND	110	89%	ND	3	22%	[8]
		ND	7.4	88%	ND	13	13%	[9]
		17	990	28%				[10]
		<1	44		<1	20		

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Antibiotics	Sulfathiazole	ND	ND	0%	ND	ND	0%	[1]
	Tetracycline	ND	ND	0%	ND	ND	0%	[5]
	Trimethoprim	0.5	6.5	83%	ND	ND	0%	[1]
		ND	18					[3]
			48	74%				[4]
		ND	20	6.8%				[5]
		ND	11	58%	ND	ND	0%	[7]
		2.2	10.9	5.8%	ND	19.8	88%	[8]
		<1	2.3		<1	1.3		[10]
	Tylosin				ND	ND	0%	[1]
		ND	ND	0%				[5]
	Virginiamycin				ND	ND	0%	[1]
		ND	ND	0%				[5]
Anticoagulants	Warfarin				ND	ND	0%	[1]
		ND	ND					[3]
Antidepressants		ND	ND	0%				[5]
	Diazepam	ND	0.47	11%	ND	0.33	6%	[7]
	Fluoxetine				ND	ND	0%	[1]
		ND	<18	1.4%				[5]
		ND	3	16%	ND	0.82	11%	[7]
		ND	0.9	38%	ND	19	13%	[8]
	Meprobamate		73	91%		43	83%	[4]
		ND	73	84%	ND	42	78%	[7]
		5.5	160	35%				[9]
		<1	16		<1	13		[10]
Antiepileptics	Carbamazepine	55	1500	100%	48	258	100%	[1]
		ND	420					[3]
			69	83%		18	61%	[4]
		ND	190	22%				[5]
		2	156					[6]
		ND	51	79%	ND	18	44%	[7]
		0.5	4.1	100%	ND	25	13%	[8]

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Antiepileptics	Carbamazepine	31	190	18%				[9]
		<1	39					[10]
	Phenytoin (Dilantin)		40	91%		32	74%	[4]
		ND	29	74%	ND	19	56%	[7]
		<1	5.3		<1	6.7		[10]
Antihistamine	Primidone	2	35					[6]
		20	54	25%				[9]
	Diphenhydramine	2	4	25%	ND	ND	0%	[1]
Antihypertensions		ND	ND					[3]
	Diphenhydramine	ND	23	5.4%				[5]
	Diltiazem				ND	ND	0%	[1]
Antioxidants		ND	ND					[3]
		ND	<12	1.4%				[5]
	Furosemide				ND	ND	0%	[1]
	5-Methyl-1H-Benzotriazole				ND	0ND	0%	[1]
	BHA				ND	ND	0%	[1]
Antipsychotics		ND	3,520	15%	ND	3,450	7%	[2]
	BHT	ND	49	5%	ND	26	6%	[7]
	Risperidone	ND	ND	0%	ND	ND	0%	[7]
	Phenol	210	600	67%	ND	ND	0%	[1]
		ND	<0.5	1.4%				[5]
Antiseptic	Triclosan	210	150	67%	ND	ND	0%	[1]
		ND	734	8%	ND	735	7%	[2]
			8.8	43%		1.2	9%	[4]
		ND	<1	8.1%				[5]
		ND	6.4	32%	ND	1.2	6%	[7]
		ND	105.8	63%	ND	60	63%	[8]
		<1	30		<1	43		[10]
	Atenolol		48	74%		26	57%	[4]
		ND	36	63%	ND	18	44%	[7]
		ND	ND	0%	ND	34	13%	[8]
β -blockers		6.1	200	27%				[9]
	Metoprolol	0.1	0.3	100%	ND	0.1	13%	[8]
		22	270	18%				[9]

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Cosmetics	Triethyl citrate (ethyl citrate)	50	80	50%	ND	62	50%	[1]
Fire Retardants	TBP	500	560	5.4%	80	100	83%	[5]
		65	90	83%				[1]
		ND	740	8.1%				[5]
	TCEP	70	160	100%	68	99	100%	[1]
			534	65%				[4]
		ND	<0.5	20%	ND	470	39%	[5]
		ND	530	53%				[7]
		ND	51.7	88%				[8]
		7.9	66	57%	<10	19		[9]
		<1	43					[10]
	TCPP		721	57%		508	48%	[4]
		ND	720	42%	ND	510	28%	[7]
	TDCPP	80	300	100%	150	250	100%	[1]
		ND	<0.5	12%				[5]
Fragrances	1,4-Dichlorobenzene	ND	<500		ND	ND	0%	[1]
								[5]
	3-methyl-1(H)-indole (Skatole)	ND	<1,000		ND	ND	0%	[1]
								[5]
	Acetophenone Galaxolide (HHCB)	45	120	92%	60	82	92%	[1]
								[4]
								[5]
								[7]
								[10]
	Tonalide (AHTN)	250	690	100%	310	490	100%	[1]
								[5]
								[5]
Lipid Regulators	Atorvastatin	ND	1.4	16%	ND	ND	0%	[7]
	Clofibrate	ND	900	15%	ND	ND	0%	[2]
	Clofibric Acid	ND	630	8%	ND	ND	0%	[2]
	Gemfibrozil	ND	ND	0%	ND	ND	0%	[1]
								[5]
								[4]
		ND	24	58%	ND	2.1	39%	[7]

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Lipid Regulators	Gemfibrozil	13	130	20%				[9]
Metabolites	Cotinine	<1	11		<1	6.5		[10]
		13	35	100%	13	25	100%	[1]
		ND	ND					[3]
		ND	100					[5]
		ND	2.7	25%	ND	0.4	13%	[8]
		13	27	18%				[9]
	Erythromycin-H ₂ O	23	700	67%	ND	ND	0%	[1]
		ND	300	8.1%				[5]
		0.3	2.7	100%	1	14	100%	[8]
	Dehydronifedipine	1	60	50%	ND	4	50%	[1]
		ND	ND					[3]
		ND	19	4.1%				[5]
		7.7	120	25%				[9]
	Nonylphenol (NP)				ND	ND	0%	[1]
			141	48%		104	17%	[4]
		ND	130	42%	ND	110	11%	[7]
		53.4	185.6	100%	12	61	100%	[8]
	Diaminochlorotriazine	10	300	62%				[9]
	Norfluoxetine	ND	ND	0%	ND	ND	0%	[7]
	NPEO ₂ -total	2500	3000	58%	ND	ND	0%	[1]
	<i>o</i> -Hydroxy Atorvastatin	ND	1.2	16%	ND	ND	0%	[7]
	<i>p</i> -Hydroxy Atorvastatin	ND	2	16%	ND	ND	0%	[7]
Muscle Relaxants	Carisoprodol	5.4	43	20%				[9]
Pesticides	2,4-D	11	23	42%				[9]
	Atrazine		1,011	87%		990	91%	[4]
		ND	870	79%	ND	930	83%	[7]
		3.4	75.1	100%	1	15	100%	[8]
	Bromacil	<1	571		<1	<1		[10]
					ND	ND	0%	[1]
		ND	740					[5]
	Chlorpyrifos	6	290	31%				[9]
					ND	ND	0%	[1]
		ND	<500					[5]

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Pesticides	DEET	68	70	25%	ND	66	25%	[1]
		ND	131	8%	ND	ND	0%	[2]
			105	48%		99	43%	[4]
		ND	<500	14%				[5]
		ND	110	32%	ND	93	33%	[7]
		23.3	255.7	100%	0.5	24	100%	[8]
		2.2	67	80%				[9]
		3.9	28		<1	30		[10]
					ND	ND	0%	[1]
		ND	510					[5]
	Dichlorvos	ND	<1,000		ND	ND	0%	[1]
								[5]
	Digoxigenin				ND	ND	0%	[1]
	Diuron	5.3	940	51%				[9]
	Linuron					8.1	17%	[4]
	Linuron	ND	9.3	26%	ND	6.2	11%	[7]
	Metolachlor				ND	ND	0%	[1]
			119	48%		36	35%	[4]
		ND	670	39%				[5]
		ND	81	37%	ND	27	33%	[7]
		<10	174		<10	160		[10]
	Pentachlorophenol	150	230	33%	ND	ND	0%	[1]
		ND	<2	5.4%				[5]
	Prometon	80	96	25%	ND	96	25%	[1]
Plasticizers	Simazine	7.1	160	77%				[9]
	Thiabendazole	ND	ND					[3]
	2-Butoxyethanol Phosphate	ND	960					[5]
	BBP	ND	1,190	15%	ND	911	33%	[2]
		ND	54	11%	ND	ND	0%	[7]
	Bisphenol A	100	300	100%	110	420	100%	[1]
		ND	1,900					[5]
		ND	14	16%	ND	25	6%	[7]
		ND	21.9	75%	ND	44	50%	[8]
	Carbaryl				ND	ND	0%	[1]

Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Plasticizers	Carbazole	80	102	17%	ND	ND	0%	[1]
	DBP	ND	8,340	31%	ND	2,730	7%	[2]
	DEHP	ND	5,940	15%	ND	2,680	13%	[2]
		ND	170	11%	ND	ND	0%	[7]
	DEP	ND	1490	15%	ND	2470	7%	[2]
	DMP	ND	784	38%	ND	54	7%	[2]
	DOP					117	35%	[4]
	TBEP	150	350	83%	150	350	83%	[1]
	Triphenyl Phosphate				ND	ND	0%	[1]
Psycho-stimulants	Caffeine	ND	<0.5	1.4%				[5]
		40	250	100%	48	119	100%	[1]
		ND	290					[3]
		ND	270	7.5%				[5]
		7	140					[6]
		ND	15.9	50%	ND	12	38%	[8]
		13	300	32%				[9]
		<10	87		<10	35		[10]
	<i>p</i> -Xanthine	ND	120					[3]
	Paraxanthine (1,7-dimethylxanthine)	90	160	75%	ND	ND	0%	[1]
		ND	300	23%				[5]
		8.9	23	18%				[9]
Steroids	Theobromine	6.4	67	35%				[9]
	17 α -ethynylestradiol	ND	1.4	5%	ND	ND	0%	[7]
	17 β -estradiol	ND	17	5%	ND	ND	0%	[7]
	β -sitosterol	850	5000	83%	ND	ND	0%	[1]
	β -stigmastanol				ND	ND	0%	[1]
		ND	<2	1.4%				[5]
	Cholesterol	800	2200	83%	ND	ND	0%	[1]
	Coprostanol	250	600	33%	ND	ND	0%	[1]
		ND	<2	18%				[5]
	Estrone (E1)		2	74%				[4]
		ND	0.9	79%	ND	ND	0%	[7]
		<1	1.4		<1	2.3		[10]

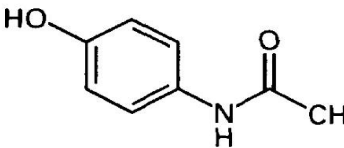
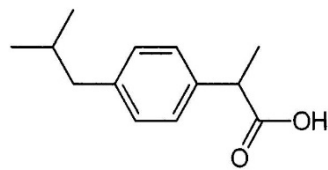
Table S7. Occurrence of CECs that have been reported in source water and finished drinking water in the United States (continued)

Groups	Compounds	Source Water (ng/L)		Freq.	Finished Drinking Water (ng/L)		Freq.	Ref.
		Minimum	Maximum	%	Minimum	Maximum	%	
Steroids	Genistein					2.9	9%	[4]
	Progesterone	ND	3.1	21%	ND	0.57	6%	[7]
	Testosterone	ND	1.2	11%	ND	ND	0%	[7]
Surfactants	4-Tert-octylphenol	ND	<1,000					[5]
	PFOA		112	76%		104	76%	[11]
			100	57%				[12]
		ND	31		ND	30		[13]
		<10	137					[14]
			100	76%	ND	4,300		[15]
	PFOS		48.3	88%		36.9	80%	[11]
			43	30%				[12]
		ND	41		ND	57		[13]
		<25	346					[14]
			400	50%	<0.25	15		[15]
	Surfynol	ND	818	31%	ND	161	27%	[2]
Sunscreens	4-n-Octylphenol				ND	ND	0%	[1]
	4-Tert-octylphenol				ND	ND	0%	[1]
	Benzophenone	50	99	58%	ND	130	58%	[1]
		ND	790	23%	ND	260	7%	[2]
	Hydrocinnamic acid	ND	20,300	23%	ND	20,100	20%	[2]
Ulcer Treatments	OMC	ND	5,610	15%	ND	45	7%	[2]
	Cimetidine				ND	ND	0%	[1]
		ND	ND	0%				[5]
	Ranitidine				ND	ND	0%	[1]
		ND	ND	0%				[5]
X-ray Contrast Media	Ioohexal	73	960	29%				[9]
	Iopromide	<1	46		<1	31		[10]

WTP – Water treatment plant; TBEP – Tri(2-butoxyethyl) phosphate; TBP – Tributyl phosphate; TCEP – Tris(2-chloroethyl) phosphate; TCPP – Tris-(2-chloroisopropyl)-phosphate; TDCPP – Tris(dichloroisopropyl) phosphate; AHAN – Acetyl-hexamethyl-tetrahydro-naphthalene; BBP – Butyl benzyl phthalate; BHA – Butylated hydroxyanisole; BHT – Butylated hydroxytoluene; NPEO2-total – 4-nonylphenol diethoxylate; DEET – N,N-diethyl-meta-toluamide; DBP – Dibutyl phthalate; DEHP – Di-(2-ethylhexyl) phthalate; DEP – Diethyl phthalate; DMP – Dimethyl phthalate; DOP – Dioctyl phthalate; OMC – Octyl methoxycinnamate; 2,4-D – 2,4-dichlorophenoxyacetic acid; PFOA – perfluorooctanoic acid; PFOS – perfluorooctanesulfonic acid.

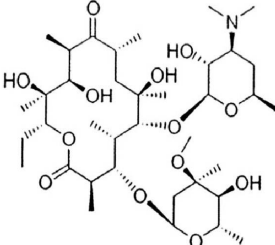
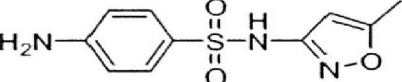
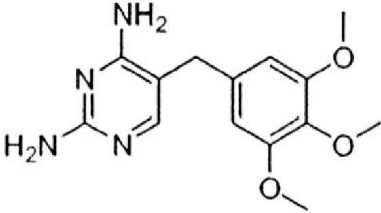
[1] Stackelberg et al., 2004; [2] Loraine et al., 2006; [3] Fram and Belitz, 2011; [4] Snyder et al., 2008; [5] Focazio et al., 2008; [6] Guo and Krasner, 2009; [7] Benotti et al., 2009; [8] Padhye et al., 2014; [9] Oppenheimer et al., 2011; [10] Snyder et al., 2007; [11] Boone et al., 2019; [12] Post et al., 2013; [13] Quiñones and Snyder, 2009; [14] Sun et al., 2016; [15] Crone et al., 2019.

Table S8. Properties of Analgesics

Analgesics	Acetaminophen	Ibuprofen
Structure ^{6,7}		
Chemical Name	N-(4-hydroxyphenyl)-acetamide	α -methyl-4-(2-methylpropyl)-benzeneacetic acid
Molecular Formula ²	C ₈ H ₉ NO ₂	C ₁₃ H ₁₈ O ₂
Aqueous Solubility ^{1,5}	Value: 1.4 $\times 10^4$ mg/L Temp: 25 °C	Value: 21 mg/L Temp: 25 °C
Boiling Point ⁸	387.8 $\pm$ 25.0 °C	319.6 $\pm$ 11.0 °C
Molecular Weight ²	151.17	206.23
Vapor Pressure ⁸	1.43 $\times 10^{-6}$ Torr Temp: 25 °C	1.39 $\times 10^{-4}$ Torr Temp: 25 °C
Log K _{ow} ³	0.46	3.97
pK _a ^{2,3}	9.38	4.91
k ₀₃ ^{9,10,12}	2.70 $\times 10^5$ M ⁻¹ s ⁻¹ (pH 7)	9.6 ($\pm$ 1) M ⁻¹ s ⁻¹ (pH 7, 20°C)
K _{OH} ^{9,10,11}	—	6.5 $\times 10^9$ -7.4 ($\pm$ 1.2) $\times 10^9$ M ⁻¹ s ⁻¹ (pH 7, 25°C)
K _{oc} ^{4,13}	170-1300 mL·g C ⁻¹	18-155 mL·g C ⁻¹
Structural Features ¹	Phenol, amide	Aromatic ring, carboxylic acid

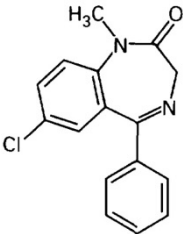
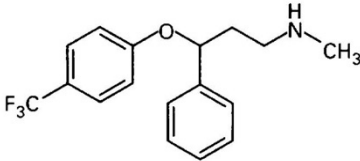
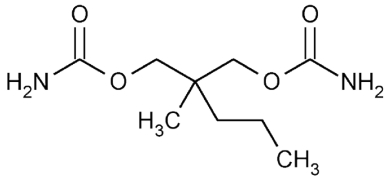
[1] Snyder et al. (2007); [2] Gros et al. (2006); [3] Schwab et al. (2005); [4] Scheytt et al., 2005; [5] DrugBank (2018); [6] Daughton (1999); [7] Tixier et al. (2003); [8] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [9] Huber et al. (2003); [10] Huber et al. (2005); [11] Nanaboina et al. (2010); [12] Javier Rivas et al. (2010); [13] Yamamoto et al., 2009.

Table S9. Properties of Antibiotics

Antibiotics	Erythromycin	Sulfamethoxazole	Trimethoprim
Structure ⁴			
Chemical Name	Erythromycin	4-amino-N-(5-methyl-3-isoxazolyl)-benzenesulfonamide	5-[(3,4,5-trimethoxyphenyl)methyl]-2,4-Pyrimidinediamine
Molecular Formula ¹	C ₃₇ H ₆₇ O ₁₃	C ₁₀ H ₁₁ N ₃ O ₃ S	C ₁₄ H ₁₈ N ₄ O ₃
Aqueous Solubility ¹	Value: 1.44 mg/L Temp: 25 °C	Value: 610 mg/L Temp: 37 °C	Value: 400 mg/L Temp: 25 °C
Boiling Point ⁵	818.4±65.0 °C	482.1±55.0 °C	526.0±60.0 °C
Molecular Weight ⁴	733.93 g/mol	253.28 g/mol	290.32 g/mol
Vapor Pressure ⁵	4.94×10 ⁻³¹ Torr Temp: 25 °C	1.89×10 ⁻⁹ Torr Temp: 25 °C	3.74×10 ⁻¹¹ Torr Temp: 25 °C
Log K _{ow} ²	3.06	0.89	0.91
pK _a ³	8.8	6.0	7.12
k ₀₃ ^{6,7,8}	—	5.5×10 ⁵ -2.5×10 ⁶ M ⁻¹ s ⁻¹ (pH 7, 20°C)	2.7×10 ⁵ M ⁻¹ s ⁻¹ (pH 7, 20°C)
K _{OH} ^{6,7}	—	5.5 (±0.7)×10 ⁹ M ⁻¹ s ⁻¹ (pH 7, 25°C)	6.9 (±0.2)×10 ⁹ M ⁻¹ s ⁻¹ (pH 7, 25°C)
K _{oc} ⁹	570 mL·g C ⁻¹	72 mL·g C ⁻¹	75 mL·g C ⁻¹
Structural Features ¹	Complex aliphatic structure, ketone, alcohols, ester, ethers, tertiary amine, heterocyclic rings	Sulfone, primary amine, secondary amine, aromatic ring, isoxazole ring	Aromatic ring, pyrimidine ring, primary amines, methoxy groups

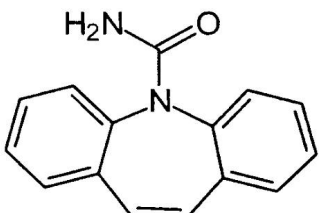
[1] Snyder et al. (2007); [2] Schwab et al. (2005); [3] Gros et al. (2006); [4] Yargeau and Leclair, (2008); [5] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [6] Huber et al. (2003); [7] Huber et al. (2005); [8] Dodd et al. (2006); [9] Hazardous Substances Data Bank (HSDB).

Table S10. Properties of Antidepressants

Antidepressants	Diazepam	Fluoxetine	Meprobamate
Structure ⁵			
Chemical Name	7-chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one	N-methyl-γ-[4-(trifluoromethyl)phenoxy]-benzenepropanamine	2-methyl-2-propylpropane-1,3-diol dicarbamate
Molecular Formula ⁵	C ₁₆ H ₁₃ ClN ₂ O	C ₁₇ H ₁₈ F ₃ NO	C ₉ H ₁₈ N ₂ O ₄
Aqueous Solubility ^{1, 7}	Value: 50 mg/L Temp: 25 °C	Value: 60.3 mg/L Temp: 25 °C	Value: 4,700 mg/L
Boiling Point ⁶	297.4±45.0 °C	395.1±42.0 °C	344.5±89.0 °C
Molecular Weight ⁵	284.74 g/mol	309.3 g/mol	218.25g/mol
Vapor Pressure ⁶	4.98×10 ⁻¹⁰ Torr Temp: 25 °C	1.88×10 ⁻⁶ Torr Temp: 25 °C	3.05×10 ⁻³ Torr Temp: 25 °C
Log K _{ow} ^{1,2,7}	2.70	2.60	0.70
pK _a ^{3,4,6}	2.4	8.7	9.2
k ₀₃ ⁸	0.75±0.15 M ⁻¹ s ⁻¹	-	-
K _{OH} ⁸	7.2 (±1.0)×10 ⁹ M ⁻¹ s ⁻¹ (pH 7, 25°C)	-	-
Structural Features ¹	Aromatics rings, heterocyclic ring, cyclic amide	Aromatic rings, secondary amine, fluorines	Aliphatic, carbamates

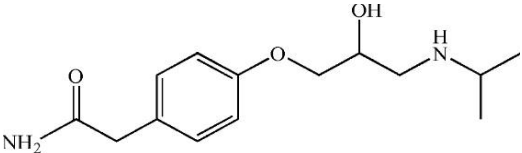
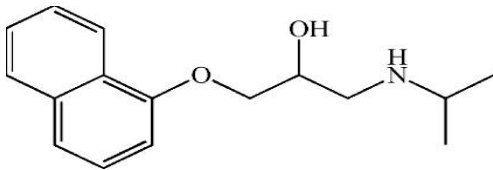
[1] Snyder et al. (2007); [2] Schwab et al. (2005); [3] Gros et al. (2006); [4] Yoon et al. (2007); [5] Daughton (1999); [6] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [7] Kwon and Armbrust, (2008); [8] Huber et al., 2003.

Table S11. Properties of Antiepileptic

Antiepileptic	Carbamazepine
Structure	
Chemical Name	5H-dibenzazepine-5-carboxamide
Molecular Formula ²	C ₁₅ H ₁₂ N ₂ O
Aqueous Solubility ¹	Value: 17.7 mg/L Temp: 25 °C
Boiling Point ⁴	411.0±48.0 °C
Molecular Weight ²	236.27 g/mol
Vapor Pressure ⁴	5.78×10 ⁻⁷ Torr Temp: 25 °C
Log K _{ow} ²	2.47
pK _a ²	7
k ₀₃ ^{5,6}	3×10 ⁵ M ⁻¹ s ⁻¹ (pH 7, 20 °C)
K _{OH} ^{5,6}	8.8 (±1.2)×10 ⁹ M ⁻¹ s ⁻¹ (pH 7, 25 °C)
K _{oc} ⁷	510 mL·g C ⁻¹
Structural Features	Aromatic rings, heterocyclic ring, amide

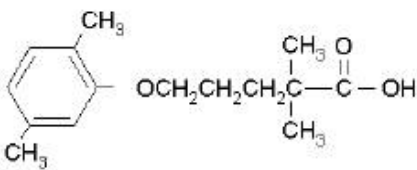
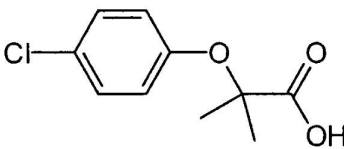
[1] Snyder et al. (2007); [2] Gros et al. (2006); [3] Tixier et al. (2003); [4] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [5] Huber et al. (2003); [6] Huber et al. (2005); [7] Hazardous Substances Data Bank (HSDB).

Table S12. Properties of β -Blockers

Beta Blockers	Atenolol	Propranolol
Structure ⁵		
Chemical Name	4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-benzeneacetamide	1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)- 2-propanol
Molecular Formula ¹	C ₁₄ H ₂₂ N ₂ O ₃	C ₁₆ H ₂₁ NO ₂
Aqueous Solubility ^{3,4}	26.7 mg/L	70 mg/L
Boiling Point ⁶	508.0±50.0 °C	434.9±30.0 °C
Molecular Weight ¹	266.34	259.80
Vapor Pressure ⁶	3.82×10 ⁻¹¹ Torr	2.48×10 ⁻⁸ Torr
Log K _{ow} ^{1,2}	Temp: 25 °C 0.16	Temp: 25 °C 3.48
pK _a ^{1,2}	9.6	9.58
k _{o3} ^{7,8}	1.7 (±0.4)×10 ³ M ⁻¹ s ⁻¹ (pH 7, 20-22 °C)	1.0×10 ⁵ M ⁻¹ s ⁻¹
K _{OH} ^{7,8}	8.0 (±0.5)×10 ⁹ M ⁻¹ s ⁻¹ (pH 7, 20-22 °C)	1.0×10 ¹⁰ M ⁻¹ s ⁻¹
K _{oc} ⁹	148-1700 mL·g C ⁻¹	—
Structural Features	Aromatic ring, carboxylic acid, ether, amine	Aromatic ring, carboxylic acid, ether, amine

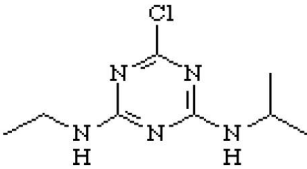
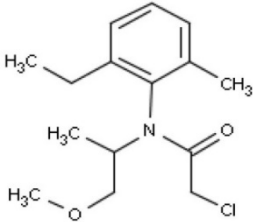
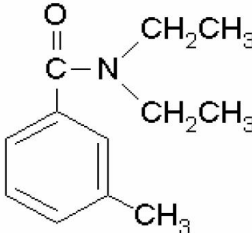
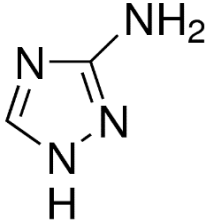
[1] Gros et al. (2006); [2] de Ridder et al. (2009); [3] Hatem et al. (1996); [4] DrugBank (2018); [5] Lavén et al. (2009); [6] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [7] Hollender et al. (2009); [8] Reungoat et al. (2010); [9] Yamamoto et al., 2009; [10] Drori et al., 2005.

Table S13. Properties of Blood Lipid Regulators

Blood Lipid Regulators	Gemfibrozil	Clofibrlic Acid
Structure ^{1,3}		
Chemical Name ²	5-(2,5-dimethylphenoxy)-2,2-dimethyl-Pentanoic acid	2-(4-chlorophenoxy)-2-methyl-propanoic acid
Molecular Formula ^{1,4}	C ₁₅ H ₂₂ O ₃	C ₁₀ H ₁₁ O ₃ Cl
Aqueous Solubility ¹	19 mg/L	Value: 583 mg/L
Boiling Point ²	394.7±30.0 °C	Temp: 25 °C
Molecular Weight ^{1,4}	250.16	324.1±17.0 °C
Vapor Pressure ²	6.13×10 ⁻⁷ Torr	214.5
Log K _{ow} ^{1,4,5}	Temp: 25 °C	1.03×10 ⁻⁴ Torr
pK _a ¹	4.77	Temp: 25 °C
k _{o3} ^{3,5}	2.88	2.88
K _{OH} ³	3.2	20 M ⁻¹ s ⁻¹
K _{oc} ⁴	2.0×10 ³ M ⁻¹ s ⁻¹	4.7×10 ⁹ M ⁻¹ s ⁻¹
Bioconcentration Factor ²	1.0×10 ¹⁰ M ⁻¹ s ⁻¹	-
Structural Features ¹	430 mL·g C ⁻¹	-
	1100-6.39 (1≤pH≤7, 25°C);	40.7-5.44 (1≤pH≤4, 25°C);
	1 (8≤pH≤10, 25°C)	1 (5≤pH≤10, 25°C)
	Aromatic ring, carboxylic acid, ether	Aromatic ring, carboxylic acid, ether

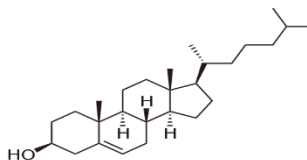
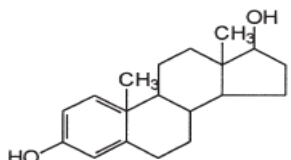
[1] Snyder et al. (2007); [2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [3] Nanaboina et al. (2010); [4] Hazardous Substances Data Bank (HSDB); [5] Huber et al. (2005).

Table S14. Properties of Pesticides

Pesticides	Atrazine	Metolachlor	DEET	Aminotriazole
Structure ¹				
Chemical Name	6-chloro-N-2-ethyl-N4-(1-methylethyl)-1,3,5-triazine-2,4-diamine	2-chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)-acetamide	N,N-diethyl-3-methylbenzamide	3-amino-1,2,4-triazole
Molecular Formula ¹	C ₈ H ₁₄ ClN ₅	C ₁₅ H ₂₂ ClNO ₂	C ₁₂ H ₁₇ NO	C ₂ H ₄ N ₄
Aqueous Solubility ^{1,2}	Value: 34.7 mg/L Temp: 26 °C	Value: 530 mg/L Temp: 20 °C	Value: 912 mg/L Temp: 25 °C	Values: 280,000 mg/L Temp: 25 °C
Boiling Point ³	368.5±25.0 °C	406.8±45.0 °C	297.5±0.0 °C	347.2±25.0 °C
Molecular Weight ¹	215.1 g/mol	283.8 g/mol	191.13 g/mol	84.08 g/mol
Vapor Pressure ³	1.27×10 ⁻⁵ Torr Temp: 25 °C	7.91×10 ⁻⁷ Torr Temp: 25 °C	1.53×10 ⁻³ Torr Temp: 25 °C	5.45×10 ⁻⁵ Torr Temp: 25 °C
Log K _{ow} ^{1,2}	2.61	3.13	2.18	-0.97
pK _a ^{1,3}	1.7	-1.34	0.67	11.14
k ₀₃ ^{4,6,7}	6.0-7.9 M ⁻¹ s ⁻¹	3.0 M ⁻¹ s ⁻¹	1.0 M ⁻¹ s ⁻¹	—
K _{OH} ^{4,5,6,7}	2.4×10 ⁹ -3.0×10 ⁹ M ⁻¹ s ⁻¹	—	5.0×10 ⁹ M ⁻¹ s ⁻¹	—
K _{oc} ^{8,9,10}	23-101 mL·g C ⁻¹	—	300 mL·g C ⁻¹	—
Structural Features ¹	Triazine ring, secondary amines, chlorine	Aromatic ring, amide, methoxy, chlorine	Aromatic ring, amide	Triazine ring, amines

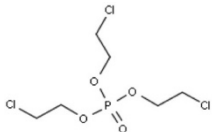
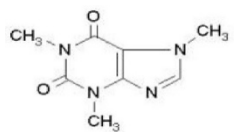
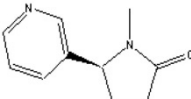
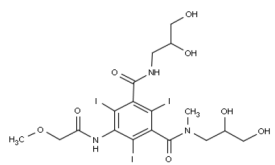
[1] Snyder et al. (2007); [2] Fontecha-Cámara et al. (2007); [3] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [4] Hollender et al. (2009); [5] Huber et al. (2003); [6] Westerhoff et al. (2005); [7] Acero et al. (2000); [8] Nkedi-Kizza et al. (2006); [9] Drori et al. (2005); [10] Hazardous Substances Data Bank (HSDB).

Table S15. Properties of Steroids

Steroids	Cholesterol	17 β -estradiol
Structure ⁶		
Chemical Name	(3 β)-cholest-5-en-3-ol	(17 β)-Estra-1,3,5(10)-triene-3,17-diol
Molecular Formula	C ₂₇ H ₄₆ O	C ₁₈ H ₂₄ O ₂
Aqueous Solubility ^{1,4,8}	Value: 0.095 mg/L Temp: 30 °C	Value: 3.6 mg/L Temp: 25 °C
Boiling Point ⁷	480.6 $\pm$ 14.0 °C	445.9 $\pm$ 45.0 °C
Molecular Weight	386.65 g/mol	272.38g/mol
Vapor Pressure ⁷	2.95 $\times$ 10 ⁻¹¹ Torr Temp: 25 °C	9.82 $\times$ 10 ⁻⁹ Torr Temp: 25 °C
Log K _{ow} ^{2,3,5,6}	8.74	4.01
pK _a ^{3,7}	15.03	10.4
k _{OH} ⁹	—	1.0 $\times$ 10 ⁶ M ⁻¹ s ⁻¹ (20 °C)
K _{OH} ⁹	—	1.41 $\times$ 10 ¹⁰ M ⁻¹ s ⁻¹
K _{oc} ^{10,11,12}	—	3700-10000 mL·g C ⁻¹
Structural Features ⁶	Alcohol, aliphatic rings	Phenol, alcohol, aliphatic rings

[1] Human Metabolome Database (2018); [2] Elkins and Mullis (2006); [3] Nghiem et al. (2004); [4] DrugBank (2018); [5] Yoon et al. (2007); [6] Snyder et al. (2007); [7] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [8] Hakk et al. (2005); [9] Broséus et al. (2009); [10] Yamamoto et al. (2005); [11] Carballa et al. (2008); [12] Karnjanapiboonwong et al. (2010).

Table S16. Properties of Other PPCPs

Compounds	TCEP	Caffeine	PFOA	PFOS	Cotinine	Iopromide
Structure ^{1,17}						
Chemical Name	2-chloro-phosphate (3:1) ethanol	3,7-dihydro-1,3,7-trimethyl-1H-Purine-2,6-dione	Perfluorooctanoic acid	Perfluorooctane sulfonic acid	1-methyl-5-(3-pyridinyl)-, (5S)-2-Pyrrolidinone	N1,N3-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-5-[(2-methoxyacetyl)amino]-N1-methyl-1,3-Benzenedicarboxamide
Molecular Formula ^{1,15}	C ₆ H ₁₂ Cl ₃ O ₄ P	C ₈ H ₁₀ N ₄ O ₂	C ₇ F ₁₅ COOH	C ₈ F ₁₇ SO ₃ H	C ₁₀ H ₁₂ N ₂ O	C ₁₈ H ₂₄ I ₃ N ₃ O ₈
Aqueous Solubility ^{1,3,4,15}	Value: 7,000 mg/L	Value: 2.16 × 10 ⁴ mg/L	Value: 2.29 × 10 ³ mg/L	Value: 3.2 × 10 ⁻³ mg/L	Value: 1.17 × 10 ⁵ mg/L	Value: 23.8 mg/L
Boiling Point ^{6,15}	347.4±0.0 °C	416.8±37.0 °C	192 °C	249 °C	316.0±0.0 °C	840.9±65.0 °C
Molecular Weight ^{1,15}	285.5 g/mol	194.1 g/mol	414.07	500.126	176.1 g/mol	791.11 g/mol
Vapor Pressure ^{6,15}	1.08×10 ⁻⁴ Torr	3.72×10 ⁻⁷ Torr	3.16×10 ⁻² mm Hg	2×10 ⁻³ mm Hg	4.21×10 ⁻⁴ Torr	5.00×10 ⁻³⁰ Torr
Temp: 25 °C	Temp: 25 °C	Temp: 25 °C	Temp: 25 °C	Temp: 25 °C	Temp: 25 °C	Temp: 25 °C
Log K _{ow} ^{1,4,15}	1.44	-0.07	4.81	4.49	0.04	-2.05
pK _a ^{1,2,4,15}	7.6	10.4	-0.5—4.2	<1	4.72	-2.60
k ₀₃ ^{7,8,9,11}	—	6.50 (±0.2)×10 ² M ⁻¹ s ⁻¹ (20 °C)	—	—	—	< 0.8 M ⁻¹ s ⁻¹ (pH 7, 20°C)
K _{OH} ^{7,8,9,10,11,12}	5.60 (±0.21)×10 ⁸ M ⁻¹ s ⁻¹	5.9×10 ⁹ -6.9×10 ⁹ M ⁻¹ s ⁻¹	—	—	—	3.3 (±0.6)×10 ⁹ M ⁻¹ s ⁻¹ (pH 7, 25°C)
K _{oc} ^{13,14,16}	67 mL·g C ⁻¹	22 mL·g C ⁻¹	29.51 mL·g C ⁻¹	125.89 mL·g C ⁻¹	130 mL·g C ⁻¹	0.005 mL·g C ⁻¹
Structural Features ¹	Phosphate, chlorines, aliphatic structure	Xanthine ring	Carbon-fluorine bond	Carbon-fluorine bond	Ketone, pyridine ring	Aromatic ring, iodines, alcohols, methoxy, amides

[1] Snyder et al. (2007); [2] Dmitrenko et al. (2007); [3] Trenholm et al. (2006); [4] Cone and Huestis (2007); [5] Human Metabolome Database (2018); [6] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs); [7] Hollender et al. (2009); [8] Huber et al. (2003); [9] Huber et al. (2005); [10] Westerhoff et al. (2005); [11] Broséus et al. (2009); [12] Watts and Linden (2009); [13] Hazardous Substances Data Bank (HSDB); [14] Carballa et al., 2008; [15] Gagliano et al., 2020; [16] Rahman et al., 2014; [17] Trojanowicz et al., 2018.

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