

**Effect of filtration on the quality of monitoring data reported for
organic compounds during wastewater treatment**

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Supplemental Tables (3)

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Table S1. Chemical Abstract Service (CAS) registry number, concentration (total and dissolved) and logarithmically transformed pH-dependent organic-water distribution coefficient (D_{OC}) of selected organic compounds reported in raw sewage. The pH values of 2 and 7.5 refer to solution pH in individual studies (indicated as X) prior to filtration.

CAS #	Compound	Ref.	Concentration (ng/L)		Log D_{OC}	
			Total	Dissolved	pH 2	pH 7.5
962-32-3	Benzo(a)anthracene, BaA				4.061	4.061
		1		3.9		X
		1		8		X
		1		35		X
		2	335			
243-17-4	Benzo(b)fluoranthene, BbF				4.312	4.312
		1		6.5		X
		1		9.3		X
		1		38		X
		2	275			
207-08-9	Benzo(k)fluoranthene, BkF				4.86	4.86
		1		34		X
		1		6.6		X
		1		11.4		X
50-32-8	Benzo(a)pyrene, BaPy				4.86	4.86
		1		4.1		X
		1		7.1		X
		1		35		X
		2	297			
131-56-6	Benzophenone-1				3.104	2.864
		3		46-400	X	
		3		51-700	X	
		4		306	X	
131-55-5	Benzophenone-2				3.104	2.864
		3		9-247	X	
		3		61-403	X	
		4		25	X	
131-57-7	Benzophenone-3				3.356	3.077
		3		<104-1068	X	
		3		<104-3975	X	
		4		971	X	
101-53-1	p-Benzylphenol				3.265	3.265
		3		<94-517	X	
		3		<94-1111	X	
		4		3578	X	
41859-67-0	Bezafibrate				3.236	0
		3		209-1391	X	
		3		135-1285	X	

		4	971	X	
		5	100-7600		X
		6	600*		X
80-05-7	Bisphenol A			3.243	3.243
		3	222-727	X	
		3	322-1163	X	
		4	540	X	
		7	210-2400		X
		8	960		X
		8	1600		X
		9	910		
		9	1142		
		10	720-3400		
		11	4761		X
		11	2520		X
		12	1620-2800	X	
		12	360-1370	X	
		12	1146-2160	X	
		13	1050		X
		13	1280		X
		13	990		X
		13	1700		X
1675-54-3	Bisphenol A diglycidyl ether, BADGE			3.526	3.526
		8	0.57		X
		8	96		X
		13	650		X
		13	640		X
		13	1150		X
		13	493		X
85-68-7	Butyl Benzyl Phthalate, BBP			4.100	4.100
		14	500		X
		14	1200		X
54208-63-8	Bisphenol F diglycidyl ether, BFDGE			3.146	3.146
		8	0.32		X
		8	89		X
		13	211		X
94-26-8	Butylparaben			3.257	3.152
		3	<2-114	X	
		3	274-1595	X	
		4	52	X	
		7	20-260		X
13171-00-1	Celestolide			4.373	4.373

		5		37.2		
120-32-1	Chlorophene				3.778	3.774
		3		27-258	X	
		3		37-141	X	
		4		114	X	
218-01-9	Chrysene				4.592	4.592
		1		5.2		X
		1		12.4		X
		1		34		X
		2	218			
23593-75-1	Clotrimazole				1.846	4.306
		5		23-33		X
84-74-2	di-n-butyl phthalate, DBP				4.000	4.000
		14		62000		X
		14		22000		X
		14		7100		X
		14		6600		X
117-81-7	di-(2-ethylhexyl) phthalate, DEHP				6.114	6.114
		14		2700		X
		14		2900		X
		14		2700		X
		14		1100		X
		14		1900		X
15307-86-5	Diclofenac				3.581	0.585
		3		26-257	X	
		3		57-1161	X	
		4		70	X	
		5		105-4110		X
		15		9.5		X
		15		13.9		X
		16		204		X
		7		50-2450		X
		6		1300*		X
		10	200-3600			
72-20-8	Endrin				4.029	4.029
		17		1.8		X
53-16-7	Estrone				3.382	3.381
		18	65.7			
		19	54.8			
		5		2.4-670		X
		16		29.5		X
		7		19207		X
57-91-0	Estradiol				3.623	3.622

50-28-2	17 β -estradiol	16		8.3		X
					3.623	3.622
		18	15.8			
		19	22			
		5		2.5-125		X
57-91-0	17 α -estradiol	7		3-22		X
					3.623	3.622
		5		1.5-17.2		X
57-63-6	17 α -ethinylestradiol				3.834	3.834
		18	8.2			
31879-05-7	Fenoprofen	5		0.4-70		X
					3.465	0.488
1222-05-5	Galaxolide	6		1800*		X
					4.767	4.767
		23	1941			
		22	390			
		5		790-4443		X
25812-30-0	Gemfibrozil	16		2031		X
					3.762	1.28
		5		700-3000		X
		15		120-36530		X
		15		181.8		X
		15		450.2		X
		15		451.3		X
		16		453		X
		7		120-36530		X
		6		700*		X
		20		25		X
76-44-8	Heptachlor				4.348	4.348
		20		46		X
1024-57-3	Heptachlor-exo-epoxide				4.352	4.352
15687-27-1	Ibuprofen	20		330		X
					3.400	0.604
		3		968-2986	X	
		3		984-6328	X	
		4		3742	X	
		5		170-83500		X
		16		8450		X
		7		4100-10210		X
		6		38700*		X

		10	34000-168000	84000		X
		21		710-1900		X
		21		550-1200		X
		21		3500-4900		X
		21		1900-2700		X
		21		1500-3800		X
		21		1400-3700		X
53-86-1	Indomethacin				3.061	0.055
		16		230		X
		7		30-430		X
193-39-5	Indeno(1,2,3-cd)pyrene, IP				5.127	5.127
		1		<1-23		X
		2	158			
61-68-7	Mefenamic acid				4.267	1.276
		3		<20-1269	X	
		3		<17-32	X	
		4		444	X	
		5		136-3200		X
22204-53-1	Naproxen				3.009	0.616
		3		400-1457	X	
		3		620-3504	X	
		4		1082	X	
		5		1790-611000		X
		16		5580		X
		7		1730-6030		X
		6		40700*		X
		21		1400-1600		X
		21		300-260		X
		21		280		X
		21		1800-1800		X
		21		1100-1300		X
		21		2200-2400		X
		21		1300-1400		X
		20		3000		X
104-40-5	4-Nonylphenol				4.745	4.745
		7		2720-25000		X
		11		2736		X
		11		2004		X
		11		8127		X
		11		285		X
		11		5155		X
		11		114		X

		9	132		
		9	10		
		9	100		
15323-35-0	Phantolide			4.534	4.534
		16	42		X
79902-63-9	Simvastatin			3.778	3.778
		3	<7-798	X	
10540-29-1	Tamoxifen			2.565	4.643
		5	143-215		X
85771-77-3	4-tert-Octylphenol			4.057	4.057
		11	745		X
		11	363		X
		3	16-558	X	
		3	<20-1151	X	
		4	465	X	
		7	380-3560		X
576-55-6	3,4,5,6-Tetrabromo-o-cresol			4.515	3.494
		3	51-1362	X	
		4	844	X	
21145-77-7	Tonalide			4.841	4.841
		22	86		
		23	583		
		5	210-1690		X
		16	804		X
68140-48-7	Traseolide			4.719	4.719
		16	168		X
3380-34-5	Triclosan			4.19	3.987
		24	1200		
		25	4800		
		3	<97-240	X	
		3	33-463	X	
		4	70	X	
		5	380		X
		16	1930		X
		7	870-1830		X
		9	2.3		
		9	16.47		
		9	1		
		10	390-4200		

137862-53-4	Valsartan			3.943	0
		3	132-1660	X	
		3	354-5388	X	
		4	676	X	
* Median concentration					

Table S2. Chemical Abstract Service (CAS) registry number and concentrations (dissolved-measured and total-computed) of organic compounds included in Figure 2. Also shown is the mass fraction in percent of chemical sorbed ($C_{\text{sorb}}(\%)$).

CAS #	Compound	Ref.	Concentration (ng/L)		$C_{\text{sorb}}(\%)$
			Dissolved	Total	
1675-54-3	Bisphenol A diglycidyl ether, BADGE	8	0.57	0.73	22
		8	96	124	22
		13	650	838	22
		13	640	825	22
		13	1150	1482	22
		13	493	635	22
15307-86-5	Diclofenac	3	26	35	25
		3	257	341	25
		3	57	76	25
		3	1161	1541	25
		3	70	93	25
		3	70	93	25
57-91-0	Estradiol	16	8.3	11.3	26
50-28-2	17 β -Estradiol	5	2.5	3.4	26
		5	125	170	26
		7	3	4	26
		7	22	30	26
57-91-0	17 α -Estradiol	5	1.5	2.0	26
120-32-1	Chlorophene	5	17.2	23.4	26
		3	27	41	34
		3	258	391	34
		3	37	56	34
		3	141	214	34
		3	114	173	34
79902-63-9	Simvastatin	3	798	1210	34
57-63-6	17 α -Ethinylestradiol	5	0.4	0.6	37
		5	70	111	37
137862-53-4	Valsartan	3	132	232	43
		3	1660	2913	43
		3	354	621	43
		3	5388	9456	43
		4	676	1186	43
		4	676	1186	43
84-74-2	di-n-butyl phthalate, DBP	14	62000	115320	46
		14	22000	40920	46
		14	7100	13206	46
		14	6600	12276	46
3380-34-5	Triclosan	5	380	697	46

		16	1930	3542	46
		7	870	1597	46
		7	1830	3358	46
72-20-8	Endrin	7	1.8	3.5	48
962-32-3	Benzo(a)anthracene, BaA	1	35	70	50
		1	8	16	50
		1	3.9	7.8	50
85771-77-3	4-tert-Octylphenol	11	745	1475	50
		11	363	719	50
		3	16	32	50
		3	558	1105	50
		3	1151	2279	50
		4	465	921	50
		7	380	753	50
		7	3560	7050	50
85-68-7	Butyl Benzyl Phthalate, BBP	14	1200	2500	52
		14	500	1042	52
3380-34-5	Triclosan	3	240	560	57
		3	33	77	57
		3	463	1080	57
		4	70	163	57
61-68-7	Mefenamic acid	3	1269	3288	61
		3	32	83	61
		4	444	1150	61
243-17-4	Benzo(b)fluoranthene, BbF	1	38	105	64
		1	9.3	25.7	64
		1	6.5	18.0	64
23593-75-1	Clotrimazole	5	23	63	64
		5	33	90	66
76-44-8	Heptachlor	5	46	134	66
1024-57-3	Celestolide	5	37.2	112.7	67
576-55-6	3,4,5,6-Tetrabromo-o-cresol	3	51	194	74
		3	1362	5192	74
		4	844	3217	74
15323-35-0	Phantolide	16	42	166	75
218-01-9	Chrysene	1	34	148	77
		1	12.4	54.1	77
		1	5.2	22.7	77
10540-29-1	Tamoxifen	5	143	683	79
		5	215	1027	79
68140-48-7	Traseolide	16	168	924	82

1222-05-5	Galaxolide	5	790	4764	83
		5	4443	26796	83
		16	2031	12249	83
104-40-5	4-Nonylphenol	7	2720	15679	83
		7	25000	144110	83
		11	2736	15771	83
		11	2004	11552	83
		11	8127	46847	83
		11	285	1643	83
		11	5155	29715	83
		11	114	657	83
207-08-9	Benzo(k)fluoranthene, BkF	1	34	246	86
		1	6.6	47.7	86
		1	11.4	82.4	86
50-32-8	Benzo(a)pyrene, BaPy	1	35	253	86
		1	7.1	51.3	86
		1	4.1	29.6	86
21145-77-7	Tonalide	5	210	1463	86
		5	1690	11777	86
		16	804	5603	86
		1	23	288	92
		14	2700	304560	99
193-39-5 117-81-7	Indeno(1,2,3-cd)pyrene, IP di-(2-ethylhexyl) phthalate, DEHP	14	2900	327120	99
		14	2700	304560	99
		14	1100	124080	99
		14	1900	214320	99

Table S3. Chemical Abstract Service (CAS) registry number and concentration spread (difference between maximum and minimum) of organic compounds before and after adjustment of concentrations from dissolved only to total estimated analyte mass present per volume.

CAS#	Compound	Ref.	Initial Conc.-C _i (ng/L)			Final Conc.-C _f (ng/L)			C _f /C _i (%)
			Min	Max	Spread	Min	Max	Spread	
50-32-8	BaPy	1	4.1	297	292.9	29.6	297	267.4	91
218-01-9	Chrysene	1	5.2	218	212.8	22.7	218	195.3	92
243-17-4	BbF	1	6.5	275	268.5	18.0	275	257	96
962-32-2	BaA	1	3.9	335	331.1	7.8	335	327.2	99
15697-27-1	Ibuprofen	3	170	168000	167830	170	168000	167830	100
53-86-1	Indomethacin	16	30	430	400	30	430	400	100
3380-34-5	Triclosan	24	1	4800	4799	1	4800	4799	100
15307-86-5	Diclofenac	3	9.5	4110	4100.5	9.5	4111	4101.5	100
22204-53-1	Naproxen	3	260	611000	610740	260	611217	610957	100
25812-30-0	Gemfibrozil	5	25	36530	36505	25	36590	36565	100
207-08-9	BkF	1	6.6	204	197.4	47.7	246	198.3	100
41859-67-0	Bezafibrate	3	135	7600	7465	100	7601	7501	100
131-56-6	Benzophenone-1	3	46	700	654	51	776	725	111
131-55-5	Benzophenone-2	3	9	403	394	10	447	437	111
54208-63-8	BFDGE	8	0.32	211	210.68	0.36	236	235.64	112
88-04-0	4-Chloroxylenol	3	4069	65381	61312	4618	74209	69591	114
80-05-7	Bisphenol A	3	210	4761	4551	241	5473	5232	115
94-26-8	Butylparaben	3	20	1595	1575	22	1843	1821	116
101-53-1	p-Benzylphenol	3	517	3578	3061	599	4144	3545	116
131-57-7	Benzophenone-3	3	52	3975	3923	62	4751	4689	120
53-16-7	Estrone	18	2.4	19207	19205	2.9	23180	23177.1	121
1675-54-3	BADGE	8	0.57	1150	1149.4	0.73	1482	1481.27	129

50-28-2	17 β -Estradiol	18	2.5	125	122.5	3.4	170	166.6	136
57-91-0	17 α -Estradiol	5	1.5	17.2	15.7	2.0	23.4	21.4	136
120-32-1	Chlorophene	3	27	258	231	41	391	350	152
79902-63-9	Simvastatin	3	4.9	798	793.1	7.43	1210	1202.57	152
57-63-6	17 α -Ethinylestradiol	18	0.4	70	69.6	0.6	111	110.4	159
137862-53-4	Valsartan	3	132	5388	5256	232	9456	9224	175
84-74-2	DBP	14	6600	62000	55400	12276	115320	103044	186
85-68-7	BBP	14	500	1200	700	1042	2500	1458	208
23593-75-1	Clotrimazole	5	23	33	10	63	90	27	270
576-55-6	3,4,5,6-Tetrabromo-o-cresol	3	51	1362	1311	194	5192	4998	381
10540-29-1	Tamoxifen	5	143	215	72	683	1027	344	478
104-40-5	4-Nonylphenol	7	10	25000	24990	10	144110	144100	577
1222-05-5	Galaxolide	23	390	4443	4053	390	26796	26406	652
21145-77-7	Tonalide	22	86	1690	1604	86	11777	11691	729
117-81-7	DEHP	14	1100	2900	1800	124080	327120	203040	11280

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