

Supplementary Material for “Insights on impact estimation of unmeasured micropollutants from WWTP release”

R. Servien, K. Bonnot, E. Latrille, A. Hélias, D. Patureau

Table S1 – List of the 40 molecular descriptors used as inputs in the predictive models (Servien et al., 2022a).

Category	Molecular descriptors		
Constitutional	Number of atoms	Number of non-H atoms	Number of hydrogen atoms
	Number of chlorine atoms	Number of carbon atoms	Number of nitrogen atoms
	Number of oxygen atoms	Number of phosphorus atoms	Number of sulfur atoms
	Number of fluorine atoms	Number of circuits	Number of halogen atoms
	Number of bonds	Number of non-H bonds	Number of double bonds
	Number of triple bonds	Number of multiple bonds	Number of rotatable bonds
	Number of aromatic bonds	Sum of conventional bond order	Number of rings
	Molecular weight		
Geometric	Connolly molecular surface area		
Topological	Connectivity index of order 0	Connectivity index of order 1	Connectivity index of order 2
	Connectivity index of	Connectivity index of	Connectivity index of order 5

	order 3	order 4	
	Valence connectivity index of order 0	Valence connectivity index of order 1	Valence connectivity index of order 2
	Valence connectivity index of order 3	Valence connectivity index of order 4	Valence connectivity index of order 5
Quantum-chemical	Polarizability	Electric dipole moment	HOMO energy
	LUMO energy	Total energy	

Table S2. Summary of the characterization factors of the 106 compounds. In the column “CF_{HT} from USEtox[®]” (resp. “CF_{ET} from USEtox[®]”), a number 1 means that the corresponding characterization factor was collected in the USEtox[®] database. If not, it was calculated using the models of Servien et al. (2022a).

CAS number	Name	Log ₁₀ CF _{HT} (DALY/kg)	CF _{HT} from		Log ₁₀ CF _{ET} (PDF.m ³ .d)	CF _{ET} from USEtox [®]
			USEtox [®]			
100-41-4	Ethylbenzene	-6.25	1		1.94	1
1024-57-3	Heptachlor epoxide	-0.09	1		5.5	1
107-06-2	1,2-dichloroethane	-4.74	1		0.88	1
108-88-3	Toluene	-7.09	1		1.45	1
111988-49-9	Thiacloprid	-5.17	0		4.11	0
111991-09-4	Nicosulfuron	-4.52	0		2.51	1
114798-26-4	Losartan	-4.01	0		3.99	0
115-29-7	Endosulfan	-4.09	1		5.47	1
118-74-1	Hexachlorobenzene	-2.04	1		4.71	1
118-79-6	2,4,6-tribromophenol	-3.73	0		4.44	1
120-12-7	Anthracene	-2.53	1		5.18	1
12002-48-1	Trichlorobenzene	-4.84	0		2.76	1
124495-18-7	Quinoxifen	-2.96	0		4.78	0
128-37-0	Butylhydroxytoluene	-5.41	1		2.95	1
131860-33-8	Azoxystrobin	-4.16	0		4.59	1
1330-20-7	Xylenes	-7.08	1		1.59	1
135410-20-7	Acetamiprid	-5.47	0		3.72	0

138261-41-3	Imidacloprid	-5.17	1	3.2	1
139968-49-3	Metaflumizone	-4.21	0	4.54	0
140-66-9	Octylphenols	-5.05	0	4.24	1
14297-93-9	4-epi-chlortetracycline	-4.46	0	3.21	0
143-50-0	Chlordecone	-1.37	1	5.77	1
153719-23-4	Thiamethoxam	-5.21	0	4.32	0
1582-09-8	Trifluralin	-4.03	1	4.73	1
15972-60-8	Alachlor	-4.97	0	4.58	1
1746-01-6	2,3,7,8-T4CDD	3.22	1	6.67	1
19408-74-3	1,2,3,7,8,9-H6CDD	-1.6	0	5.25	0
2032-65-7	Methiocarb	-5.12	1	4.96	1
20427-84-3	NP2EO	-5.13	0	3.99	0
210880-92-5	Clothianidin	-5.25	0	3.52	0
21312-10-7	Acetyl sulfamethoxazole	-5.49	0	3.92	0
2303-17-5	Triallate	-4.37	1	3.97	1
2315-61-9	OP2EO	-5.09	0	3.96	0
2315-67-5	OP1EO	-5.11	0	4.19	0
2385-85-5	Mirex	-1.61	1	2.93	1
25167-80-0	Monochlorophenol	-5.34	0	3.18	0
25167-82-2	Trichlorophenols	-4.6	0	3.01	1
25167-83-3	Tetrachlorophenols	-4.15	0	4.93	1
28159-98-0	Cybutryne	-5.11	0	6.01	1
2921-88-2	Chlorpyrifos	-2.91	1	6.49	1
302-01-2	Hydrazine	-3.51	1	4.14	1
309-00-2	Aldrin	-1.48	1	5.13	1
32536-52-0	Octabromodiphenylethers	-2.57	0	5.25	0
32598-13-3	PCB 77	-2.9	0	4.08	1
32598-14-4	PCB 105	-2.53	0	6.06	0
3268-87-9	1,2,3,4,6,7,8,9-O8CDD	-1.38	0	5.25	0
32774-16-6	PCB 169	-1.85	0	6.53	0

330-55-2	Linuron	-4	1	5	1
3424-82-6	DDE 24'	-3.06	0	5.2	0
35822-46-9	1,2,3,4,6,7,8-H7CDD	-1.48	0	5.25	0
36355-01-8	Hexabromobiphenyl	-2.02	0	5.25	0
36483-60-0	Hexabromodiphenylethers	-1.97	0	5.25	0
38380-08-4	PCB 156	-2.06	0	6.43	0
39001-02-0	1,2,3,4,6,7,8,9-O8CDF	-1.1	0	5.25	0
39227-28-6	1,2,3,4,7,8-H6CDD	-1.52	0	5.25	0
39635-31-9	PCB 189	-1.65	0	5.25	0
40321-76-4	1,2,3,7,8-P5CDD	-1.85	0	8.76	1
42576-02-3	Bifenox	-4.77	0	5.04	1
446255-20-5	Heptabromodiphenylethers	-2.34	0	5.25	0
470-90-6	Chlorfenvinphos	-2.54	1	5	1
49690-94-0	Tribromodiphenylethers	-3.44	0	5.29	0
50-29-3	DDT 44'	-2.18	1	5.14	1
50-32-8	Benzo(a)pyrene	-1.5	1	3.93	1
51207-31-9	2,3,7,8-T4CDF	-2.19	0	8.65	1
52663-72-6	PCB 167	-2.01	0	6.48	0
53-19-0	DDD 24'	-10	1	5.24	0
5466-77-3	Octinoxate	-5.44	0	3.87	0
55673-89-7	1,2,3,4,7,8,9-H7CDF	-1.46	0	5.25	0
56-23-5	Carbon tetrachloride	-4.28	1	1.51	1
564-25-0	Doxycycline	-4.38	0	4.42	0
57-62-5	Chlortetracycline	-4.49	0	2.64	1
57-74-9	Chlordane	-0.92	1	4.96	1
57117-31-4	2,3,4,7,8-P5CDF	-1.79	0	5.25	0
57117-41-6	1,2,3,7,8-P5CDF	-1.67	0	5.25	0
57117-44-9	1,2,3,6,7,8-H6CDF	-1.62	0	5.25	0
57465-28-8	PCB 126	-2.44	0	6.13	0
57653-85-7	1,2,3,6,7,8-H6CDD	-1.51	0	6.18	1

58-89-9	Lindane	-2.91	1	5.16	1
60-57-1	Dieldrin	-0.82	1	5.49	1
608-73-1	Hexachlorocyclohexane	-3.12	1	4.84	1
608-93-5	Pentachlorobenzene	-3.57	1	3.92	1
60851-34-5	2,3,4,6,7,8-H6CDF	-1.73	0	5.25	0
615-58-7	2,4-dibromophenol	-4.44	0	3.76	0
62-53-3	Aniline	-5	1	2.5	1
65510-44-3	PCB 123	-2.58	0	5.94	0
66108-95-0	Iohexol	-4.96	0	0.61	0
67-56-1	Methanol	-7.55	1	0.12	1
67562-39-4	1,2,3,4,6,7,8-H7CDF	-1.5	0	5.25	0
69782-90-7	PCB 157	-2.33	0	6.13	0
70362-50-4	PCB 81	-2.96	0	5.62	0
70648-26-9	1,2,3,4,7,8-H6CDF	-1.61	0	5.25	0
71-43-2	Benzene	-5.59	1	1.52	1
72-20-8	Endrin	-1.72	1	6.77	1
72-54-8	DDD 44'	-0.45	1	6.13	1
72-55-9	DDE 44'	-2.38	1	5.55	1
72918-21-9	1,2,3,7,8,9-H6CDF	-1.56	0	5.25	0
73334-07-3	Iopromide	-6.2	1	1.08	1
74472-37-0	PCB 114	-2.43	0	6.11	0
75-01-4	Chloroethene	-4.46	1	2.68	0
76-44-8	Heptachlor	-1.67	1	4.83	1
789-02-6	DDT 24'	-2.5	0	4.99	1
79-01-6	Trichloroethylene	-6.35	1	1.62	1
8001-35-2	Toxaphene	-0.65	1	5.72	1
87-68-3	Hexachlorobutadiene	-3.81	1	3.58	1
87-86-5	Pentachlorophenols	-3.42	1	4.66	1
95-56-7	2-bromophenol	-5.12	0	2.55	1

Table S3. Summary of the concentration measurements of the 106 compounds, from Aemig et al. (2021). When a measurement is below the LOQ, the usual estimation of LOQ/2 is applied. Note that, for some measurements in the literature, the concentrations are reported without the LOQ.

CAS number	Name	Mean concentration ($\mu\text{g.L}^{-1}$)	Maximal concentration ($\mu\text{g.L}^{-1}$)	Percentage of measurements above LOQ (%)	LOQ ($\mu\text{g.L}^{-1}$)	Number of sites of measurements
100-41-4	Ethylbenzene	0.5	0.5	0	1	87
1024-57-3	Heptachlor epoxide	0.01	0.01	0	0.02	3
107-06-2	1,2-dichloroethane	1.06	2.5	1	2	742
108-88-3	Toluene	0.51	1.7	9	0.1	87
111988-49-9	Thiacloprid	NA	NA	NA	NA	NA
111991-09-4	Nicosulfuron	0.025	0.025	0	0.05	4
114798-26-4	Losartan	0.17	0.7	63	NA	8
115-29-7	Endosulfan	0.012	1.5	5	0.02	728
118-74-1	Hexachlorobenzene	0.0057	1.2	1	0.01	749
118-79-6	2,4,6-tribromophenol	NA	NA	NA	NA	0
120-12-7	Anthracene	0.021	0.4	4	0.04	751
12002-48-1	Trichlorobenzene	0.108	4	3	0.2	749
124495-18-7	Quinoxifen	0.05	0.05	0	0.1	3
128-37-0	Butylhydroxytoluene	NA	NA	NA	NA	NA
131860-33-8	Azoxystrobin	NA	NA	NA	NA	NA
1330-20-7	Xylenes	1.04	4	2	2	87
135410-20-7	Acetamiprid	NA	NA	NA	NA	NA
138261-41-3	Imidacloprid	0.025	0.025	0	0.05	3
139968-49-3	Metaflumizone	NA	NA	NA	NA	NA
140-66-9	Octylphenols	0.05	0.5	10	0.1	736
14297-93-9	4-epi-chlortetracycline	NA	NA	NA	NA	NA
143-50-0	Chlordecone	0.1	0.1	0	0.2	85

153719-23-4	Thiamethoxam	NA	NA	NA	NA	NA
1582-09-8	Trifluralin	0.0057	1	5	0.01	746
15972-60-8	Alachlor	0.0116	3.4	1	0.02	748
1746-01-6	2,3,7,8-T4CDD	NA	NA	NA	NA	NA
19408-74-3	1,2,3,7,8,9-H6CDD	NA	NA	NA	NA	NA
2032-65-7	Methiocarb	NA	NA	NA	NA	NA
20427-84-3	NP2EO	0.16	0.8	9	0.3	796
210880-92-5	Clothianidin	NA	NA	NA	NA	NA
21312-10-7	Acetyl sulfamethoxazole	NA	NA	NA	NA	NA
2303-17-5	Triallate	NA	NA	NA	NA	NA
2315-61-9	OP2EO	0.05	0.7	8	0.1	754
2315-67-5	OP1EO	0.06	10.1	6	0.1	756
2385-85-5	Mirex	0.0259	0.1	4	0.05	84
25167-80-0	Monochlorophenol	NA	NA	NA	NA	0
25167-82-2	Trichlorophenols	NA	NA	NA	NA	0
25167-83-3	Tetrachlorophenols	NA	NA	NA	NA	0
28159-98-0	Cybutryne	NA	NA	NA	NA	NA
2921-88-2	Chlorpyrifos	0.012	14.2	5	0.02	746
302-01-2	Hydrazine	51.59	175.3	1	100	83
309-00-2	Aldrin	0.0298	29	4	0.05	746
32536-52-0	Octabromodiphenylethers	0.021	0.025	0	0.05	18
32598-13-3	PCB 77	0.0025	0.0025	0	0.005	3
32598-14-4	PCB 105	0.0025	0.0025	0	0.005	3
3268-87-9	1,2,3,4,6,7,8,9-O8CDD	NA	NA	NA	NA	NA
32774-16-6	PCB 169	0.0025	0.0025	0	0.005	3
330-55-2	Linuron	0.056	1.2	5	0.1	746
3424-82-6	DDE 24'	0.05	0.05	0	0.1	745
35822-46-9	1,2,3,4,6,7,8-H7CDD	NA	NA	NA	NA	NA
36355-01-8	Hexabromobiphenyl	0.011	0.1	4	0.02	84
36483-60-0	Hexabromodiphenylethers	0.002	0.01	0	0.003	18

38380-08-4	PCB 156	0.0025	0.0025	0	0.005	3
39001-02-0	1,2,3,4,6,7,8,9-O8CDF	NA	NA	NA	NA	NA
39227-28-6	1,2,3,4,7,8-H6CDD	NA	NA	NA	NA	NA
39635-31-9	PCB 189	0.0025	0.0025	0	0.005	3
40321-76-4	1,2,3,7,8-P5CDD	NA	NA	NA	NA	NA
42576-02-3	Bifenox	0.05	0.05	0	0.1	3
446255-20-5	Heptabromodiphenylethers	NA	NA	NA	NA	NA
470-90-6	Chlorfenvinphos	0.0548	0.5	5	0.1	748
49690-94-0	Tribromodiphenylethers	0.001	0.06	0	0.001	18
50-29-3	DDT 44'	0.0298	29	5	0.05	745
50-32-8	Benzo(a)pyrene	0.0057	1.2	4	0.01	753
51207-31-9	2,3,7,8-T4CDF	NA	NA	NA	NA	NA
52663-72-6	PCB 167	0.0025	0.0025	0	0.005	3
53-19-0	DDD 24'	0.05	0.05	0	0.1	745
5466-77-3	Octinoxate	NA	NA	NA	NA	NA
55673-89-7	1,2,3,4,7,8,9-H7CDF	NA	NA	NA	NA	NA
56-23-5	Carbon tetrachloride	0.504	0.7	1	1	746
564-25-0	Doxycycline	NA	NA	NA	NA	NA
57-62-5	Chlortetracycline	NA	NA	NA	NA	NA
57-74-9	Chlordane	0.011	0.1	1	0.02	85
57117-31-4	2,3,4,7,8-P5CDF	NA	NA	NA	NA	NA
57117-41-6	1,2,3,7,8-P5CDF	NA	NA	NA	NA	NA
57117-44-9	1,2,3,6,7,8-H6CDF	NA	NA	NA	NA	NA
57465-28-8	PCB 126	0.0025	0.0025	0	0.005	3
57653-85-7	1,2,3,6,7,8-H6CDD	NA	NA	NA	NA	NA
58-89-9	Lindane	0.0123	0.6	6	0.02	515
60-57-1	Dieldrin	0.0298	29	4	0.05	746
608-73-1	Hexachlorocyclohexane	0.01	0.01	8	0.02	100
608-93-5	Pentachlorobenzene	0.0059	3.5	1	0.01	749
60851-34-5	2,3,4,6,7,8-H6CDF	NA	NA	NA	NA	NA

615-58-7	2,4-dibromophenol	NA	NA	NA	NA	0
62-53-3	Aniline	25	25	0	50	84
65510-44-3	PCB 123	0.0025	0.0025	0	0.005	3
66108-95-0	Iohexol	2.146	120	75	NA	8
67-56-1	Methanol	5000	5000	6	10000	85
67562-39-4	1,2,3,4,6,7,8-H7CDF	NA	NA	NA	NA	NA
69782-90-7	PCB 157	0.0025	0.0025	0	0.005	3
70362-50-4	PCB 81	0.0025	0.0025	0	0.005	3
70648-26-9	1,2,3,4,7,8-H6CDF	NA	NA	NA	NA	NA
71-43-2	Benzene	0.5	1	0.1	0.1	71
72-20-8	Endrin	0.0298	29	4	0.05	746
72-54-8	DDD 44'	NA	NA	NA	NA	NA
72-55-9	DDE 44'	NA	NA	NA	NA	NA
72918-21-9	1,2,3,7,8,9-H6CDF	NA	NA	NA	NA	NA
73334-07-3	Iopromide	1.102	78.2	100	NA	8
74472-37-0	PCB 114	0.0025	0.0025	0	0.005	3
75-01-4	Chloroethene	2.5	2.5	0	5	84
76-44-8	Heptachlor	0.0105	0.03	1	0.02	90
789-02-6	DDT 24'	NA	NA	NA	NA	NA
79-01-6	Trichloroethylene	0.275	3	4	0.5	744
8001-35-2	Toxaphene	0.0269	0.5	6	0.05	56
87-68-3	Hexachlorobutadiene	0.268	4	3	0.5	746
87-86-5	Pentachlorophenols	0.056	1	9	0.1	736
95-56-7	2-bromophenol	NA	NA	NA	NA	0

Table S4 – Summary of the values of the aquatic environment characterization factor CF_{ET} (in $PDF.m^3.d$) and the human health characterization factor CF_{HT} (in $DALY.kg^{-1}$) for the compounds in the different studies.

	$\log_{10}(CF_{HT}+1e-10)$			$\log_{10}(CF_{ET})$		
	Aemig et al. (2021) n=94	Servien et al. (2022b) n=59	Added compounds n=106	Aemig et al. (2021) n=88	Servien et al. (2022b) n=65	Added compounds n=106
Maximum	-1.69	-1.69	3.22	8.05	7.21	8.76
3 rd Quartile	-3.48	-3.48	-1.81	4.70	5.25	5.25
Mean	-5.36	-4.12	-3.37	3.78	4.27	4.52
Median	-5.39	-4.36	-3.10	3.56	4.03	4.96
1 st Quartile	-6.16	-4.98	-4.93	2.70	3.86	3.88
Minimum	-10.00	-5.69	-10.00	0.86	2.07	0.12

Table S5 – Estimation of the concentrations needed to reach 1% of the global impacts on ecotoxicity, ordered by increasing percentage of RSDE LOQ. The probability is calculated when the percentage of LOQ is under 100%. It is computed using the distribution of subsection 3.2 and is the estimation that a measurement under the LOQ is above the minimal concentration.

CAS number	Name	Minimal concentration ($\mu g.L^{-1}$)	Minimal concentration (% of RSDE LOQ)	Probability
302-01-2	Hydrazine	4,0E+00	3.96	0.96
72-20-8	Endrin	1,0E-02	18.63	0.75
143-50-0	Chlordecone	9,0E-02	46.17	0.29
2921-88-2	Chlorpyrifos	2,0E-02	88.18	0.04
8001-35-2	Toxaphene	1,0E-01	208.35	NA
49690-94-0	Tribromodiphenylethers	2,8E-01	234.07	NA
53-19-0	DDD 24'	3,2E-01	319.42	NA
32774-16-6	PCB 169	2,0E-02	322.42	NA
62-53-3	Aniline	1,7E+02	347.8	NA
3424-82-6	DDE 24'	3,5E-01	349.13	NA
60-57-1	Dieldrin	1,8E-01	354.59	NA

52663-72-6	PCB 167	2,0E-02	364.43	NA
38380-08-4	PCB 156	2,0E-02	404.27	NA
67-56-1	Methanol	4,2E+04	415.7	NA
42576-02-3	Bifenox	5,0E-01	497.92	NA
470-90-6	Chlorfenvinphos	5,5E-01	551.31	NA
330-55-2	Linuron	5,5E-01	553.51	NA
32536-52-0	Octabromodiphenylethers	3,1E-01	620.85	NA
50-29-3	DDT 44'	3,9E-01	789.35	NA
69782-90-7	PCB 157	4,0E-02	809.75	NA
57465-28-8	PCB 126	4,0E-02	810.12	NA
309-00-2	Aldrin	4,1E-01	821.09	NA
74472-37-0	PCB 114	4,0E-02	857.86	NA
1024-57-3	Heptachlor epoxide	1,7E-01	866.01	NA
124495-18-7	Quinoxifen	9,0E-01	903.09	NA
120-12-7	Anthracene	3,6E-01	910.8	NA
115-29-7	Endosulfan	1,8E-01	924.54	NA
32598-14-4	PCB 105	5,0E-02	966.86	NA
87-86-5	Pentachlorophenols	1,2E+00	1212.43	NA
65510-44-3	PCB 123	6,0E-02	1249.44	NA
36355-01-8	Hexabromobiphenyl	3,1E-01	1552.13	NA
36483-60-0	Hexabromodiphenylethers	3,1E-01	1552.13	NA
20427-84-3	NP2EO	5,7E+00	1889.37	NA
58-89-9	Lindane	3,8E-01	1904.01	NA
75-01-4	Chloroethene	1,2E+02	2309.37	NA
70362-50-4	PCB 81	1,3E-01	2612.85	NA
87-68-3	Hexachlorobutadiene	1,4E+01	2869.63	NA
57-74-9	Chlordane	6,0E-01	2996.55	NA
140-66-9	Octylphenols	3,2E+00	3156.53	NA
114798-26-4	Losartan	5,6E+00	3285.2	NA
2315-67-5	OP1EO	3,5E+00	3520.9	NA

608-73-1	Hexachlorocyclohexane	7,9E-01	3930.36	NA
76-44-8	Heptachlor	8,2E-01	4083.92	NA
2315-61-9	OP2EO	6,0E+00	5977.67	NA
39635-31-9	PCB 189	3,1E-01	6208.38	NA
15972-60-8	Alachlor	1,4E+00	7219.03	NA
1582-09-8	Trifluralin	1,0E+00	10218.05	NA
118-74-1	Hexachlorobenzene	1,1E+00	10717.33	NA
12002-48-1	Trichlorobenzene	9,6E+01	48190.67	NA
50-32-8	Benzo(a)pyrene	6,5E+00	65077.11	NA
608-93-5	Pentachlorobenzene	6,6E+00	65918.81	NA
138261-41-3	Imidacloprid	3,4E+01	68741.6	NA
1330-20-7	Xylenes	1,4E+03	70955.67	NA
32598-13-3	PCB 77	4,5E+00	90874.48	NA
2385-85-5	Mirex	6,4E+01	127945.96	NA
56-23-5	Carbon tetrachloride	1,7E+03	167969.36	NA
79-01-6	Trichloroethylene	1,3E+03	264629.68	NA
111991-09-4	Nicosulfuron	1,7E+02	337930.86	NA
107-06-2	1,2-dichloroethane	7,3E+03	363822.72	NA
73334-07-3	Iopromide	4,6E+03	415421.77	NA
66108-95-0	Iohexol	1,3E+04	626838.34	NA
100-41-4	Ethylbenzene	6,3E+02	628347.54	NA
71-43-2	Benzene	1,7E+03	1665651.11	NA
108-88-3	Toluene	2,0E+03	1965008.59	NA

Table S6 – Estimation of the concentrations needed to reach 1% of the global impacts on human toxicity, ordered by increasing percentage of RSDE LOQ. The probability is calculated when the percentage of LOQ is under 100%. It is computed using the distribution of subsection 3.2 and is the estimation that a measurement under the LOQ is above the minimal concentration. When the probability is equal to one, it means that no measured value is below this percentage of LOQ. For the DDD 24' the minimal concentration is infinite because its CF_{HT} is equal to zero.

CAS number	Name	Minimal concentration ($\mu\text{g.L}^{-1}$)	Minimal concentration (% of RSDE LOQ)	Probability
302-01-2	Hydrazine	2,1E-01	0.21	1
1024-57-3	Heptachlor epoxide	8,2E-05	0.41	1
8001-35-2	Toxaphene	2,9E-04	0.59	1
143-50-0	Chlordecone	1,6E-03	0.78	1
60-57-1	Dieldrin	4,4E-04	0.88	1
57-74-9	Chlordane	5,5E-04	2.75	0.97
309-00-2	Aldrin	2,0E-03	4.04	0.96
2385-85-5	Mirex	2,7E-03	5.42	0.94
72-20-8	Endrin	3,5E-03	7.01	0.91
62-53-3	Aniline	6,6E+00	13.24	0.79
76-44-8	Heptachlor	3,1E-03	15.46	0.77
50-29-3	DDT 44'	1,0E-02	20.26	0.71
50-32-8	Benzo(a)pyrene	2,1E-03	20.77	0.7
470-90-6	Chlorfenvinphos	2,3E-02	22.83	0.67
67-56-1	Methanol	2,4E+03	23.59	0.67
36483-60-0	Hexabromodiphenylethers	6,2E-03	31.23	0.52
36355-01-8	Hexabromobiphenyl	6,9E-03	34.57	0.44
75-01-4	Chloroethene	1,9E+00	38.33	0.42
32536-52-0	Octabromodiphenylethers	2,5E-02	49.68	0.26
120-12-7	Anthracene	2,3E-02	56.45	0.18
39635-31-9	PCB 189	2,9E-03	58.63	0.18
124495-18-7	Quinoxifen	6,0E-02	59.92	0.18
118-74-1	Hexachlorobenzene	7,2E-03	72.48	0.12

3424-82-6	DDE 24'	7,6E-02	75.91	0.11
87-68-3	Hexachlorobutadiene	4,3E-01	86.26	0.06
32774-16-6	PCB 169	4,7E-03	94.43	0.02
56-23-5	Carbon tetrachloride	1,3E+00	125.9	NA
52663-72-6	PCB 167	6,8E-03	136.39	NA
38380-08-4	PCB 156	7,6E-03	152.82	NA
49690-94-0	Tribromodiphenylethers	1,8E-01	153.79	NA
87-86-5	Pentachlorophenols	1,8E-01	175.3	NA
107-06-2	1,2-dichloroethane	3,7E+00	184.02	NA
2921-88-2	Chlorpyrifos	5,4E-02	268.05	NA
58-89-9	Lindane	5,4E-02	270.92	NA
66108-95-0	Iohexol	6,0E+00	279.17	NA
69782-90-7	PCB 157	1,4E-02	281.41	NA
74472-37-0	PCB 114	1,8E-02	354.42	NA
57465-28-8	PCB 126	1,8E-02	368.87	NA
114798-26-4	Losartan	6,8E-01	398.04	NA
608-73-1	Hexachlorocyclohexane	8,7E-02	432.7	NA
32598-14-4	PCB 105	2,3E-02	453.93	NA
65510-44-3	PCB 123	2,5E-02	498.35	NA
330-55-2	Linuron	6,7E-01	667.18	NA
32598-13-3	PCB 77	5,2E-02	1046.73	NA
70362-50-4	PCB 81	6,0E-02	1196.61	NA
12002-48-1	Trichlorobenzene	4,6E+00	2281.08	NA
608-93-5	Pentachlorobenzene	2,5E-01	2475.91	NA
20427-84-3	NP2EO	8,9E+00	2961.94	NA
42576-02-3	Bifenox	3,9E+00	3907.2	NA
115-29-7	Endosulfan	8,2E-01	4087.52	NA
111991-09-4	Nicosulfuron	2,2E+00	4387.81	NA
1582-09-8	Trifluralin	7,1E-01	7131.71	NA
140-66-9	Octylphenols	7,4E+00	7397.51	NA

2315-61-9	OP2EO	8,1E+00	8109.51	NA
2315-67-5	OP1EO	8,6E+00	8566	NA
73334-07-3	Iopromide	1,0E+02	9464.13	NA
138261-41-3	Imidacloprid	9,8E+00	19603.79	NA
71-43-2	Benzene	2,6E+01	25978.17	NA
79-01-6	Trichloroethylene	1,5E+02	29490.95	NA
15972-60-8	Alachlor	6,2E+00	30777.96	NA
1330-20-7	Xylenes	8,0E+02	39767.14	NA
100-41-4	Ethylbenzene	1,2E+02	118689.1	NA
108-88-3	Toluene	8,1E+02	810430.14	NA
53-19-0	DDD 24'	Inf	Inf	NA