

Improved impact assessment of micropollutants release from WWTP

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Supplementary Material

Table S1. Summary of the aquatic environmental impact of the 153 compounds, ordered by decreasing impact. In the column “Already present”, a number 1 means that the compound was already taken into account in impact assessment of Aemig et al. (2021). The aquatic environment characterization factor CF_{ET} is expressed in $PDF.m^3.d$ (Potentially Disappeared Fraction per kg). This metric accounts for a fraction of species richness that may be potentially lost.

CAS Number	Name	Already present	Impact (%)	Emitted mass (%)	Emitted mass (kg)	CF_{ET} ($PDF.m^3.d$)	PDF (unitless)
52315-07-8	Cypermethrin	1	77,155	0,473	696,332	2,51E+07	1,75E+10
50-28-2	17- β -estradiol	1	4,758	0,007	9,610	1,12E+08	1,08E+09
154-21-2	Lincomycin	0	3,971	0,306	450,000	2,00E+06	9,01E+08
42399-41-7	Diltiazem	0	2,535	0,024	35,000	1,64E+07	5,75E+08
26787-78-0	Amoxicillin	1	2,330	0,068	100,000	5,28E+06	5,28E+08
3194-55-6	1,2,5,6,9,10-Hexabromocyclododecane	1	1,211	0,201	296,216	9,27E+05	2,75E+08
74070-46-5	Aclonifen	1	0,953	0,444	653,508	3,31E+05	2,16E+08
58-93-5	Hydrochlorothiazide	0	0,876	4,636	6821,993	2,91E+04	1,99E+08
188425-85-6	Boscalid	1	0,858	0,218	320,750	6,06E+05	1,95E+08
66357-35-5	Ranitidine	0	0,573	6,796	10000,000	1,30E+04	1,30E+08
1118-46-3	Butyltrichlorotin	1	0,470	0,713	1048,993	1,02E+05	1,07E+08
62-73-7	Dichlorvos	1	0,424	0,181	265,769	3,62E+05	9,62E+07
35065-27-1	PCB 153	0	0,260	0,012	17,649	3,34E+06	5,89E+07
115-32-2	Dicofol	1	0,259	0,166	243,790	2,41E+05	5,87E+07

58-25-3	Chlordiazepoxide	0	0,215	3,398	5000,000	9,77E+03	4,88E+07
83380-47-6	Ofloxacin	1	0,205	0,609	896,281	5,20E+04	4,66E+07
54-31-9	Furosemide	0	0,172	2,110	3105,405	1,26E+04	3,90E+07
35065-28-2	PCB 138	0	0,159	0,012	17,126	2,11E+06	3,61E+07
40487-42-1	Pendimethalin	1	0,158	0,107	156,969	2,29E+05	3,59E+07
19666-30-9	Oxadiazon	1	0,150	0,072	106,526	3,20E+05	3,41E+07
465-73-6	Isodrin	1	0,147	0,037	54,862	6,08E+05	3,34E+07
104-35-8	2-(4-Nonylphenoxy)ethanol (NP1EO)	1	0,130	0,557	819,100	3,61E+04	2,95E+07
58-08-2	Caffeine	1	0,117	0,518	762,937	3,49E+04	2,66E+07
83905-01-5	Azithromycin	1	0,111	0,340	500,000	5,01E+04	2,51E+07
31508-00-6	PCB 118	0	0,108	0,011	16,718	1,47E+06	2,45E+07
57-91-0	17- α -estradiol	1	0,080	0,005	7,732	2,34E+06	1,81E+07
34123-59-6	Isoproturon	1	0,067	0,179	263,689	5,78E+04	1,52E+07
103577-45-3	Lansoprazole	0	0,058	1,019	1500,000	8,79E+03	1,32E+07
604-75-1	Oxazepam	0	0,058	0,896	1317,730	9,92E+03	1,31E+07
301669-82-9	4-OH-omeprazole	0	0,057	1,019	1500,000	8,59E+03	1,29E+07
105827-78-9	Imidacloprid	1	0,054	0,100	146,846	8,37E+04	1,23E+07
76824-35-6	Famotidine	0	0,052	0,204	300,000	3,93E+04	1,18E+07
330-54-1	Diuron	1	0,049	0,253	372,948	3,00E+04	1,12E+07
81103-11-9	Clarithromycin	1	0,049	0,482	709,799	1,57E+04	1,11E+07
57-63-6	17- α -ethinylestradiol	0	0,049	0,005	7,047	1,57E+06	1,11E+07
205-99-2	Benzo(b)fluoranthene	0	0,048	0,042	61,861	1,77E+05	1,09E+07
134237-51-7	hexabromocyclododecane (1R,2R,5S,6R,9S,10R)-1,2,5,6,9,10-	0	0,047	0,041	60,803	1,77E+05	1,08E+07
134237-50-6	Hexabromocyclododecane (R,R,S,R,R,S)-1,2,5,6,9,10-	0	0,047	0,041	60,583	1,77E+05	1,07E+07
134237-52-8	γ -Hexabromocyclododecane	0	0,047	0,041	60,323	1,77E+05	1,07E+07
107534-96-3	Tebuconazole	1	0,045	0,203	299,115	3,43E+04	1,03E+07
35693-99-3	PCB 52	0	0,045	0,011	16,469	6,16E+05	1,02E+07
193-39-5	Indeno(1,2,3-cd)pyrene	0	0,043	0,038	55,474	1,77E+05	9,82E+06

36734-19-7	Iprodione	1	0,043	0,214	314,339	3,11E+04	9,79E+06
886-50-0	Terbutryne	1	0,042	0,199	292,771	3,22E+04	9,43E+06
207-08-9	Benzo(k)fluoranthene	0	0,041	0,036	52,696	1,77E+05	9,32E+06
32534-81-9	Pentabromodiphenylethers	1	0,039	0,008	12,503	7,14E+05	8,93E+06
36507-30-9	Carbamazepine epoxide	0	0,037	0,974	1433,155	5,80E+03	8,32E+06
1763-23-1	Perfluorooctane sulfonate (PFOS)	0	0,035	0,184	270,699	2,90E+04	7,85E+06
191-24-2	Benzo(g,h,i)perylene	0	0,035	0,030	44,277	1,77E+05	7,84E+06
25154-52-3	Nonylphenol	1	0,034	0,662	973,759	8,01E+03	7,80E+06
148-79-8	Thiabendazole	1	0,024	0,215	316,648	1,70E+04	5,38E+06
3380-34-5	Triclosan	1	0,021	0,050	73,367	6,60E+04	4,84E+06
66722-44-9	Bisoprolol	0	0,021	0,289	424,642	1,14E+04	4,82E+06
737-31-5	Diatrizoate	0	0,020	0,031	45,000	9,91E+04	4,46E+06
1912-24-9	Atrazine	1	0,018	0,063	92,772	4,37E+04	4,05E+06
36894-69-6	Labetalol	0	0,018	0,340	500,000	8,09E+03	4,04E+06
137862-53-4	Valsartan	0	0,017	17,715	26067,407	1,52E+02	3,96E+06
1066-51-9	AMPA	0	0,017	3,817	5616,686	6,85E+02	3,85E+06
121552-61-2	Cyprodinil	1	0,017	0,183	269,422	1,40E+04	3,78E+06
42200-33-9	Nadolol	1	0,016	0,014	20,828	1,79E+05	3,72E+06
122-34-9	Simazine	1	0,015	0,061	89,749	3,89E+04	3,49E+06
25637-99-4	1,3,5,7,9,11-Hexabromocyclododecane	0	0,015	0,201	296,216	1,12E+04	3,33E+06
114-07-8	Erythromycin	1	0,014	0,209	306,827	1,07E+04	3,28E+06
50-27-1	Estriol	0	0,014	0,012	18,369	1,77E+05	3,26E+06
723-46-6	Sulfamethoxazole	1	0,014	0,903	1329,044	2,35E+03	3,12E+06
138402-11-6	Irbesartan	0	0,013	8,052	11848,650	2,58E+02	3,06E+06
35065-29-3	PCB 180	0	0,013	0,011	16,310	1,77E+05	2,89E+06
1401-69-0	Tylosine	0	0,011	0,100	147,236	1,76E+04	2,60E+06
58-55-9	Theophylline	0	0,010	0,515	758,245	2,93E+03	2,22E+06
81093-37-0	Pravastatin	1	0,009	0,321	472,871	4,51E+03	2,13E+06
668-34-8	Triphenyl tin	0	0,009	0,008	11,759	1,77E+05	2,08E+06
57-41-0	Phenytoin	0	0,009	0,306	450,000	4,42E+03	1,99E+06

206-44-0	Fluoranthene	1	0,009	0,023	34,468	5,70E+04	1,96E+06
25812-30-0	Gemfibrozil	0	0,008	0,134	197,801	9,58E+03	1,89E+06
51481-61-9	Cimetidine	0	0,007	0,136	200,000	7,85E+03	1,57E+06
40088-47-9	Tetrabromodiphenylethers	0	0,007	0,004	5,269	2,89E+05	1,52E+06
15307-86-5	Diclofenac	1	0,006	1,014	1492,245	9,72E+02	1,45E+06
85721-33-1	Ciprofloxacin	1	0,006	0,407	598,393	2,28E+03	1,36E+06
525-66-6	Propranolol	1	0,005	0,436	642,235	1,85E+03	1,19E+06
70458-96-7	Norfloxacin	1	0,005	0,198	291,621	3,88E+03	1,13E+06
98-54-4	Butylphenol	1	0,005	0,322	473,688	2,32E+03	1,10E+06
54910-89-3	Fluoxetine	1	0,005	0,027	40,348	2,54E+04	1,02E+06
3115-49-9	(4-Nonylphenoxy)acetic acid (NP1EC)	1	0,004	2,097	3086,104	3,07E+02	9,47E+05
25167-81-1	2,3-dichlorophenol	1	0,004	0,184	270,513	3,47E+03	9,38E+05
101-21-3	Chlorprophame	1	0,004	0,219	322,157	2,74E+03	8,84E+05
51384-51-1	Metoprolol	1	0,004	0,331	487,128	1,76E+03	8,57E+05
125-33-7	Primidone	0	0,004	0,162	238,581	3,55E+03	8,46E+05
80-05-7	Bisphenol A	1	0,004	0,134	197,737	4,18E+03	8,26E+05
129-00-0	Pyrene	1	0,004	0,001	1,275	6,47E+05	8,25E+05
57-68-1	Sulfamethazine	0	0,004	0,076	111,440	7,36E+03	8,20E+05
298-46-4	Carbamazepine	1	0,003	1,349	1984,342	3,90E+02	7,73E+05
151602-49-2	5-O-Desmethyl Omeprazole	0	0,003	0,068	100,000	7,21E+03	7,21E+05
22071-15-4	Ketoprofen	1	0,003	0,657	967,478	7,28E+02	7,04E+05
83881-51-0	Cetirizine	0	0,003	1,019	1500,000	4,59E+02	6,89E+05
37680-73-2	PCB 101	1	0,003	0,032	47,063	1,37E+04	6,44E+05
117-81-7	Diethylhexyl phthalate (DEHP)	1	0,003	2,465	3627,379	1,61E+02	5,84E+05
67129-08-2	Metazachlor	1	0,002	0,101	148,798	3,72E+03	5,54E+05
127-18-4	Tetrachloroethylene	1	0,002	1,137	1672,868	3,03E+02	5,08E+05
7012-37-5	PCB 28	0	0,002	0,012	17,047	2,93E+04	4,99E+05
93413-69-5	Venlafaxine	1	0,002	0,646	950,095	4,69E+02	4,45E+05
15545-48-9	Chlortoluron	1	0,002	0,223	328,248	1,34E+03	4,41E+05
1088-11-5	Nordazepam	0	0,002	0,034	50,489	7,97E+03	4,02E+05

1812-30-2	Bromazepam	0	0,002	0,014	21,213	1,89E+04	4,02E+05
94-74-6	2,4 MCPA	1	0,002	0,263	386,690	9,40E+02	3,64E+05
218-01-9	Chrysene	0	0,002	0,005	7,500	4,81E+04	3,61E+05
738-70-5	Trimethoprim	1	0,002	0,482	709,932	4,98E+02	3,53E+05
92-52-4	Biphenyl	1	0,002	0,211	310,592	1,10E+03	3,42E+05
53-16-7	Estrone	1	0,002	0,020	28,895	1,18E+04	3,42E+05
50-78-2	Aspirin	0	0,002	0,087	127,398	2,68E+03	3,41E+05
56-55-3	Benzo(a)anthracene	1	0,001	0,000	0,500	6,77E+05	3,38E+05
41859-67-0	Bezafibrate	1	0,001	0,351	516,996	6,43E+02	3,33E+05
73590-58-6	Omeprazole	0	0,001	0,031	45,797	7,24E+03	3,31E+05
18559-94-9	Salbutamol	0	0,001	0,019	27,358	9,32E+03	2,55E+05
1071-83-6	Glyphosate	1	0,001	0,990	1456,127	1,60E+02	2,34E+05
80214-83-1	Roxithromycin	1	0,001	0,134	197,548	1,17E+03	2,31E+05
53-86-1	Indomethacin	0	0,001	0,639	940,151	2,08E+02	1,95E+05
61-82-5	Aminotriazole	1	0,001	0,262	385,257	4,90E+02	1,89E+05
6452-71-7	Oxprenolol	0	0,001	0,013	19,435	8,76E+03	1,70E+05
29122-68-7	Atenolol	1	0,001	1,083	1594,016	1,03E+02	1,64E+05
91-20-3	Naphthalene	1	0,001	0,233	342,872	4,53E+02	1,55E+05
83164-33-4	Diflufenicanil	1	0,001	0,120	176,358	8,48E+02	1,50E+05
3930-20-9	Sotalol	1	0,001	2,916	4291,113	3,33E+01	1,43E+05
85-01-8	Phenanthrene	1	0,001	0,012	17,000	8,21E+03	1,40E+05
94-75-7	2,4 D	1	0,001	0,219	322,215	4,30E+02	1,39E+05
26839-75-8	Timolol	0	0,001	0,008	11,882	1,06E+04	1,26E+05
22204-53-1	Naproxen	1	0,001	0,428	630,090	1,90E+02	1,20E+05
23031-25-6	Terbutaline	0	0,001	0,011	15,844	7,18E+03	1,14E+05
75-09-2	Dichloromethane	1	0,000	10,212	15026,948	7,30E+00	1,10E+05
63659-18-7	Betaxolol	0	0,000	0,007	10,258	1,06E+04	1,09E+05
28981-97-7	Alprazolam	0	0,000	0,006	8,715	1,22E+04	1,06E+05
37148-27-9	Clenbuterol	0	0,000	0,003	3,914	2,51E+04	9,81E+04
126-73-8	Tributyl phosphate	1	0,000	0,117	171,746	5,70E+02	9,78E+04

50-48-6	Amitriptyline	1	0,000	0,042	61,775	1,41E+03	8,70E+04
37517-30-9	Acebutolol	1	0,000	0,594	873,928	9,43E+01	8,24E+04
95-16-9	Benzothiazole	1	0,000	0,427	627,691	1,24E+02	7,80E+04
83915-83-7	Lisinopril	0	0,000	0,204	300,000	2,29E+02	6,87E+04
67-66-3	Trichloromethane	1	0,000	1,964	2890,451	2,06E+01	5,95E+04
108-62-3	Metalddehyde	1	0,000	0,327	480,708	1,23E+02	5,91E+04
69-72-7	Salicylic acid	1	0,000	0,385	566,980	8,03E+01	4,55E+04
50-49-7	Imipramine	0	0,000	0,004	5,294	8,03E+03	4,25E+04
15687-27-1	Ibuprofen	1	0,000	0,214	314,364	1,17E+02	3,67E+04
25057-89-0	Bentazone	1	0,000	0,214	315,062	1,00E+02	3,15E+04
1668-19-5	Doxepin	0	0,000	0,004	6,280	4,33E+03	2,72E+04
1163-19-5	Decabromodiphenylether	0	0,000	0,150	220,612	1,17E+02	2,59E+04
208-96-8	Acenaphthylene	0	0,000	0,003	5,000	4,44E+03	2,22E+04
50-06-6	Phenobarbital	1	0,000	0,340	500,000	4,04E+01	2,02E+04
86-73-7	Fluorene	1	0,000	0,006	8,500	1,80E+03	1,53E+04
73573-88-3	Mevastatin	0	0,000	0,034	50,000	2,97E+02	1,49E+04
439-14-5	Diazepam	1	0,000	0,011	15,738	8,67E+02	1,36E+04
103-90-2	Acetaminophen	1	0,000	0,203	297,996	4,33E+01	1,29E+04
83-32-9	Acenaphthene	1	0,000	0,003	4,000	2,17E+03	8,69E+03
53-70-3	Dibenzo(a,h)anthracene	1	0,000	0,002	2,500	3,05E+03	7,63E+03
14488-53-0	Butane,tin(2+)	0	0,000	0,008	11,421	2,56E+02	2,92E+03

Table S2 – List of the 40 molecular descriptors.

Category	Molecular descriptors		
Constitutional	Number of atoms	Number of non-H	Number of hydrogen

		atoms	atoms
	Number of hydrogen 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 chlorine atoms	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
	Number of circuits	Molecular weight (g/mol)	
Geometric	Connolly molecular surface area (\AA^2)		

Topological	Connectivity index of order 0	Connectivity index of order 1	Connectivity index of order 2
	Connectivity index of order 3	Connectivity index of order 4	Connectivity index of order 5
	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 (\AA^3)	Electric dipole moment (D)	HOMO energy (eV)
	LUMO energy (eV)	Total energy (eV)	

Table S3. Summary of the human health impacts of the 153 compounds, ordered by decreasing impact. In the column “Already present”, a number 1 means that the compound was already taken into account in impact assessment of Aemig et al. (2021). The human health characterization factor CF_{HT} is expressed in $\text{DALY}\cdot\text{kg}^{-1}$ (Disability Adjusted Life Year per kg). It represents the number of years lost with illness, handicap or premature death and considered both carcinogenic and non-carcinogenic effects.

CAS Number	Name	Already present	Impact (%)	Emitted mass (%)	Emitted mass (kg)	CF_{HT} (DALY/kg)	DALY
53-86-1	Indomethacin	1	25,774	0,639	940,151	7,51E-03	7,06E+00
205-99-2	Benzo(b)fluoranthene	1	18,343	0,042	61,861	8,12E-02	5,02E+00
115-32-2	Dicofol	1	16,334	0,166	243,790	1,84E-02	4,47E+00

207-08-9	Benzo(k)fluoranthene	1	6,672	0,036	52,696	3,47E-02	1,83E+00
137862-53-4	Valsartan	0	6,226	17,715	26067,407	6,54E-05	1,71E+00
193-39-5	Indeno(1,2,3-cd)pyrene	1	3,942	0,038	55,474	1,95E-02	1,08E+00
138402-11-6	Irbesartan	0	2,747	8,052	11848,650	6,35E-05	7,52E-01
15307-86-5	Diclofenac	1	2,331	1,014	1492,245	4,28E-04	6,39E-01
465-73-6	Isodrin	0	1,884	0,037	54,862	9,41E-03	5,16E-01
25637-99-4	1,3,5,7,9,11-Hexabromocyclododecane	0	1,689	0,201	296,216	1,56E-03	4,63E-01
53-70-3	Dibenzo(a,h)anthracene	1	1,317	0,002	2,500	1,44E-01	3,61E-01
32534-81-9	Pentabromodiphenylethers	1	1,288	0,008	12,503	2,82E-02	3,53E-01
35065-29-3	PCB 180	0	1,210	0,011	16,310	2,03E-02	3,31E-01
58-25-3	Chlordiazepoxide	0	0,797	3,398	5000,000	4,37E-05	2,18E-01
103577-45-3	Lansoprazole	0	0,795	1,019	1500,000	1,45E-04	2,18E-01
886-50-0	Terbutryne	1	0,669	0,199	292,771	6,26E-04	1,83E-01
35065-27-1	PCB 153	0	0,634	0,012	17,649	9,85E-03	1,74E-01
50-06-6	Phenobarbital	1	0,476	0,340	500,000	2,61E-04	1,30E-01
37680-73-2	PCB 101	0	0,454	0,032	47,063	2,64E-03	1,24E-01
134237-51-7	° -Hexabromocyclododecane	0	0,446	0,041	60,803	2,01E-03	1,22E-01
35065-28-2	PCB 138	0	0,427	0,012	17,126	6,83E-03	1,17E-01
62-73-7	Dichlorvos	1	0,402	0,181	265,769	4,14E-04	1,10E-01
218-01-9	Chrysene	1	0,345	0,005	7,500	1,26E-02	9,46E-02
134237-52-8	γ-Hexabromocyclododecane	0	0,312	0,041	60,323	1,42E-03	8,56E-02
19666-30-9	Oxadiazon	1	0,292	0,072	106,526	7,50E-04	7,99E-02
604-75-1	Oxazepam	1	0,286	0,896	1317,730	5,95E-05	7,84E-02
134237-50-6	(R,R,S,R,R,S)-1,2,5,6,9,10-Hexabromocyclododecane	0	0,285	0,041	60,583	1,29E-03	7,82E-02
36507-30-9	Carbamazepine epoxide	0	0,246	0,974	1433,155	4,70E-05	6,73E-02
57-63-6	17-α-ethinylestradiol	0	0,204	0,005	7,047	7,95E-03	5,60E-02
114-07-8	Erythromycin	0	0,197	0,209	306,827	1,76E-04	5,41E-02
31508-00-6	PCB 118	0	0,195	0,011	16,718	3,20E-03	5,35E-02
66357-35-5	Ranitidine	0	0,195	6,796	10000,000	5,35E-06	5,35E-02

206-44-0	Fluoranthene	1	0,128	0,023	34,468	1,01E-03	3,50E-02
75-09-2	Dichloromethane	1	0,123	10,212	15026,948	2,25E-06	3,37E-02
83881-51-0	Cetirizine	0	0,121	1,019	1500,000	2,21E-05	3,32E-02
191-24-2	Benzo(g,h,i)perylene	1	0,118	0,030	44,277	7,31E-04	3,24E-02
1401-69-0	Tylosine	0	0,114	0,100	147,236	2,12E-04	3,12E-02
61-82-5	Aminotriazole	1	0,098	0,262	385,257	6,96E-05	2,68E-02
94-74-6	2,4 MCPA	1	0,096	0,263	386,690	6,81E-05	2,63E-02
104-35-8	2-(4-Nonylphenoxy)ethanol (NP1EO)	0	0,090	0,557	819,100	3,01E-05	2,46E-02
1066-51-9	AMPA	0	0,083	3,817	5616,686	4,05E-06	2,27E-02
57-91-0	17- α -estradiol	1	0,076	0,005	7,732	2,71E-03	2,09E-02
3380-34-5	Triclosan	0	0,076	0,050	73,367	2,84E-04	2,08E-02
67-66-3	Trichloromethane	1	0,072	1,964	2890,451	6,79E-06	1,96E-02
35693-99-3	PCB 52	0	0,065	0,011	16,469	1,09E-03	1,79E-02
125-33-7	Primidone	1	0,064	0,162	238,581	7,35E-05	1,75E-02
737-31-5	Diatrizoate	0	0,063	0,031	45,000	3,84E-04	1,73E-02
40088-47-9	Tetrabromodiphenylethers	0	0,057	0,004	5,269	2,98E-03	1,57E-02
41859-67-0	Bezafibrate	1	0,057	0,351	516,996	3,01E-05	1,56E-02
3115-49-9	(4-Nonylphenoxy)acetic acid (NP1EC)	0	0,054	2,097	3086,104	4,82E-06	1,49E-02
117-81-7	Diethylhexyl phthalate (DEHP)	1	0,054	2,465	3627,379	4,09E-06	1,48E-02
57-41-0	Phenytoin	1	0,054	0,306	450,000	3,29E-05	1,48E-02
127-18-4	Tetrachloroethylene	1	0,053	1,137	1672,868	8,68E-06	1,45E-02
298-46-4	Carbamazepine	1	0,046	1,349	1984,342	6,29E-06	1,25E-02
668-34-8	Triphenyl tin	0	0,045	0,008	11,759	1,06E-03	1,24E-02
36894-69-6	Labetalol	0	0,045	0,340	500,000	2,44E-05	1,22E-02
54-31-9	Furosemide	1	0,042	2,110	3105,405	3,73E-06	1,16E-02
301669-82-9	4-OH-omeprazole	0	0,040	1,019	1500,000	7,37E-06	1,11E-02
66722-44-9	Bisoprolol	0	0,034	0,289	424,642	2,17E-05	9,19E-03
52315-07-8	Cypermethrin	1	0,028	0,473	696,332	1,11E-05	7,72E-03
36734-19-7	Iprodione	1	0,027	0,214	314,339	2,35E-05	7,37E-03
83164-33-4	Diflufenicanil	0	0,026	0,120	176,358	4,07E-05	7,17E-03

25812-30-0	Gemfibrozil	1	0,026	0,134	197,801	3,59E-05	7,11E-03
122-34-9	Simazine	1	0,025	0,061	89,749	7,54E-05	6,77E-03
85-01-8	Phenanthrene	1	0,024	0,012	17,000	3,91E-04	6,65E-03
330-54-1	Diuron	1	0,024	0,253	372,948	1,77E-05	6,60E-03
154-21-2	Lincomycin	0	0,024	0,306	450,000	1,46E-05	6,58E-03
83915-83-7	Lisinopril	0	0,023	0,204	300,000	2,10E-05	6,30E-03
107534-96-3	Tebuconazole	1	0,022	0,203	299,115	2,03E-05	6,08E-03
74070-46-5	Aclonifen	0	0,021	0,444	653,508	8,84E-06	5,78E-03
121552-61-2	Cyprodinil	0	0,020	0,183	269,422	2,01E-05	5,41E-03
738-70-5	Trimethoprim	1	0,019	0,482	709,932	7,50E-06	5,32E-03
151602-49-2	5-O-Desmethyl Omeprazole	0	0,019	0,068	100,000	5,26E-05	5,26E-03
1912-24-9	Atrazine	1	0,018	0,063	92,772	5,40E-05	5,01E-03
94-75-7	2,4 D	1	0,018	0,219	322,215	1,55E-05	5,00E-03
56-55-3	Benzo(a)anthracene	1	0,016	0,000	0,500	8,59E-03	4,30E-03
7012-37-5	PCB 28	0	0,016	0,012	17,047	2,51E-04	4,29E-03
105827-78-9	Imidacloprid	1	0,015	0,100	146,846	2,72E-05	4,00E-03
108-62-3	Metaldehyde	0	0,014	0,327	480,708	8,03E-06	3,86E-03
67129-08-2	Metazachlor	0	0,012	0,101	148,798	2,27E-05	3,38E-03
1763-23-1	Perfluorooctane sulfonate (PFOS)	0	0,012	0,184	270,699	1,17E-05	3,16E-03
101-21-3	Chlorprophame	1	0,011	0,219	322,157	9,55E-06	3,08E-03
91-20-3	Naphthalene	1	0,010	0,233	342,872	8,16E-06	2,80E-03
15545-48-9	Chlortoluron	0	0,010	0,223	328,248	8,32E-06	2,73E-03
93413-69-5	Venlafaxine	1	0,010	0,646	950,095	2,78E-06	2,64E-03
53-16-7	Estrone	0	0,008	0,020	28,895	7,60E-05	2,20E-03
95-16-9	Benzothiazole	0	0,007	0,427	627,691	3,11E-06	1,95E-03
25167-81-1	2,3-dichlorophenol	0	0,007	0,184	270,513	7,13E-06	1,93E-03
723-46-6	Sulfamethoxazole	1	0,006	0,903	1329,044	1,27E-06	1,69E-03
42399-41-7	Diltiazem	0	0,006	0,024	35,000	4,38E-05	1,53E-03
76824-35-6	Famotidine	0	0,005	0,204	300,000	4,92E-06	1,48E-03
26787-78-0	Amoxicillin	0	0,005	0,068	100,000	1,37E-05	1,37E-03

22204-53-1	Naproxen	1	0,005	0,428	630,090	2,00E-06	1,26E-03
3194-55-6	1,2,5,6,9,10-Hexabromocyclododecane	1	0,004	0,201	296,216	4,12E-06	1,22E-03
148-79-8	Thiabendazole	1	0,004	0,215	316,648	3,74E-06	1,18E-03
69-72-7	Salicylic acid	0	0,004	0,385	566,980	2,04E-06	1,15E-03
25057-89-0	Bentazone	1	0,004	0,214	315,062	3,29E-06	1,04E-03
50-48-6	Amitriptyline	1	0,004	0,042	61,775	1,67E-05	1,03E-03
34123-59-6	Isoproturon	0	0,004	0,179	263,689	3,69E-06	9,73E-04
525-66-6	Propranolol	1	0,003	0,436	642,235	1,48E-06	9,47E-04
25154-52-3	Nonylphenol	1	0,003	0,662	973,759	9,30E-07	9,06E-04
1812-30-2	Bromazepam	0	0,003	0,014	21,213	4,21E-05	8,92E-04
73573-88-3	Mevastatin	0	0,003	0,034	50,000	1,78E-05	8,89E-04
51384-51-1	Metoprolol	1	0,002	0,331	487,128	1,38E-06	6,71E-04
86-73-7	Fluorene	1	0,002	0,006	8,500	7,74E-05	6,58E-04
29122-68-7	Atenolol	1	0,002	1,083	1594,016	4,12E-07	6,57E-04
1071-83-6	Glyphosate	1	0,002	0,990	1456,127	4,33E-07	6,30E-04
3930-20-9	Sotalol	1	0,002	2,916	4291,113	1,41E-07	6,06E-04
129-00-0	Pyrene	1	0,002	0,001	1,275	4,71E-04	6,01E-04
80-05-7	Bisphenol A	1	0,002	0,134	197,737	2,96E-06	5,85E-04
73590-58-6	Omeprazole	1	0,002	0,031	45,797	1,26E-05	5,79E-04
50-49-7	Imipramine	0	0,002	0,004	5,294	1,06E-04	5,60E-04
85721-33-1	Ciprofloxacin	1	0,002	0,407	598,393	7,10E-07	4,25E-04
1668-19-5	Doxepin	0	0,001	0,004	6,280	6,06E-05	3,80E-04
208-96-8	Acenaphthylene	1	0,001	0,003	5,000	7,20E-05	3,60E-04
126-73-8	Tributyl phosphate	1	0,001	0,117	171,746	1,96E-06	3,37E-04
83-32-9	Acenaphthene	1	0,001	0,003	4,000	8,15E-05	3,26E-04
63659-18-7	Betaxolol	0	0,001	0,007	10,258	3,08E-05	3,16E-04
103-90-2	Acetaminophen	1	0,001	0,203	297,996	1,04E-06	3,10E-04
18559-94-9	Salbutamol	1	0,001	0,019	27,358	9,50E-06	2,60E-04
1163-19-5	Decabromodiphenylether	1	0,001	0,150	220,612	1,16E-06	2,57E-04
40487-42-1	Pendimethalin	1	0,001	0,107	156,969	1,58E-06	2,48E-04

81093-37-0	Pravastatin	1	0,001	0,321	472,871	4,82E-07	2,28E-04
92-52-4	Biphenyl	1	0,001	0,211	310,592	6,78E-07	2,11E-04
37148-27-9	Clenbuterol	0	0,001	0,003	3,914	4,73E-05	1,85E-04
57-68-1	Sulfamethazine	1	0,001	0,076	111,440	1,24E-06	1,38E-04
80214-83-1	Roxithromycin	1	0,000	0,134	197,548	6,66E-07	1,31E-04
26839-75-8	Timolol	0	0,000	0,008	11,882	9,30E-06	1,11E-04
83380-47-6	Ofloxacin	1	0,000	0,609	896,281	1,18E-07	1,06E-04
70458-96-7	Norfloxacin	1	0,000	0,198	291,621	3,54E-07	1,03E-04
6452-71-7	Oxprenolol	0	0,000	0,013	19,435	5,19E-06	1,01E-04
54910-89-3	Fluoxetine	1	0,000	0,027	40,348	2,32E-06	9,37E-05
81103-11-9	Clarithromycin	1	0,000	0,482	709,799	1,14E-07	8,11E-05
1088-11-5	Nordazepam	1	0,000	0,034	50,489	1,53E-06	7,71E-05
83905-01-5	Azithromycin	1	0,000	0,340	500,000	1,19E-07	5,97E-05
37517-30-9	Acebutolol	1	0,000	0,594	873,928	5,19E-08	4,53E-05
42200-33-9	Nadolol	1	0,000	0,014	20,828	1,83E-06	3,81E-05
14488-53-0	Butane,tin(2+)	0	0,000	0,008	11,421	3,21E-06	3,66E-05
23031-25-6	Terbutaline	1	0,000	0,011	15,844	9,70E-07	1,54E-05
188425-85-6	Boscalid	1	0,000	0,218	320,750	2,98E-08	9,57E-06
50-27-1	Estriol	1	0,000	0,012	18,369	4,54E-07	8,34E-06
28981-97-7	Alprazolam	1	0,000	0,006	8,715	9,47E-07	8,25E-06
1118-46-3	Butyltrichlorotin	1	0,000	0,713	1048,993	7,86E-09	8,24E-06
15687-27-1	Ibuprofen	1	0,000	0,214	314,364	0,00E+00	0,00E+00
22071-15-4	Ketoprofen	1	0,000	0,657	967,478	0,00E+00	0,00E+00
439-14-5	Diazepam	1	0,000	0,011	15,738	0,00E+00	0,00E+00
50-28-2	17- β -estradiol	1	0,000	0,007	9,610	0,00E+00	0,00E+00
50-78-2	Aspirin	1	0,000	0,087	127,398	0,00E+00	0,00E+00
51481-61-9	Cimetidine	1	0,000	0,136	200,000	0,00E+00	0,00E+00
58-08-2	Caffeine	1	0,000	0,518	762,937	0,00E+00	0,00E+00
58-55-9	Theophylline	1	0,000	0,515	758,245	0,00E+00	0,00E+00
58-93-5	Hydrochlorothiazide	1	0,000	4,636	6821,993	0,00E+00	0,00E+00

98-54-4 Butylphenol 1 0,000 0,322 473,688 0,00E+00 0,00E+00

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 of Aemig et al. (2021) and for the compounds studied in this work.

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