The fate of trace organic contaminants in sewage sludge during anaerobic digestion: a pilot scale study

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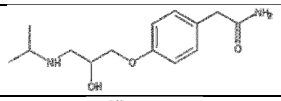
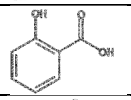
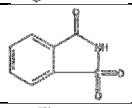
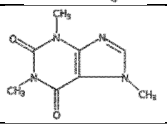
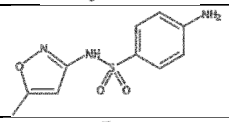
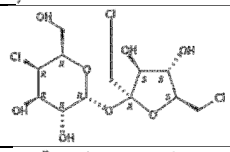
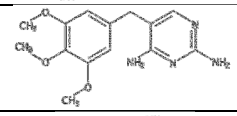
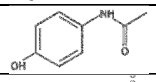
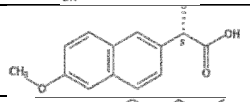
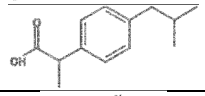
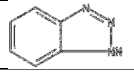
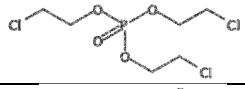
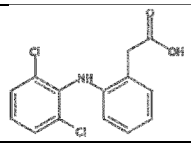
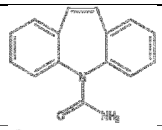
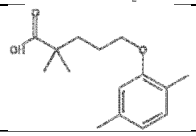
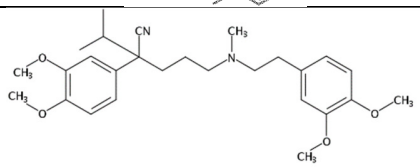
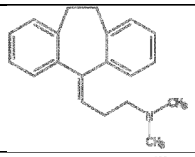
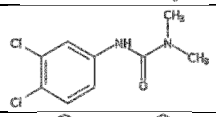
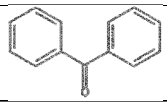
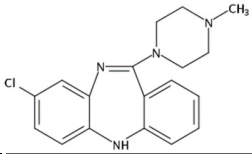
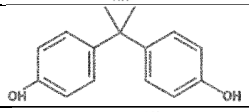
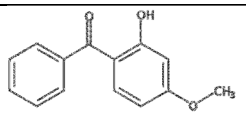
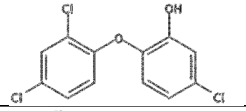
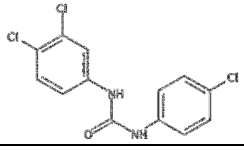
Table S1: Physicochemical properties of the 44 trace organic compounds monitored in this study.

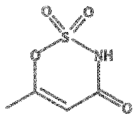
(A) 24 compounds detected in the primary sludge

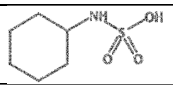
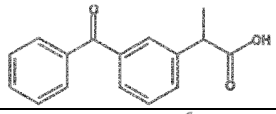
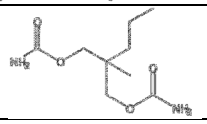
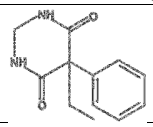
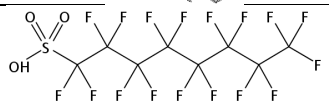
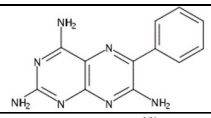
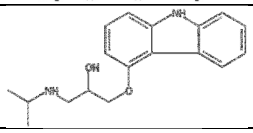
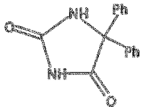
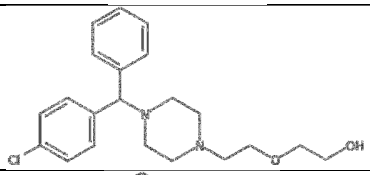
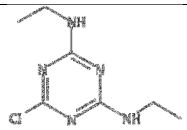
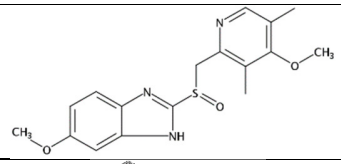
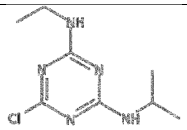
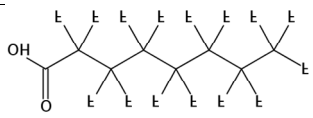
Compounds	Log D at pH=5	Log D at pH=7	MW (g/mol)	pKa	Molecular structure
Atenolol ($C_{14}H_{22}N_2O_3$)	-2.75	-2.09	266.34	13.88±0.20	
Salicyclic acid ($C_7H_6O_3$)	-0.65	-1.13	138.12	3.01±0.10	
Saccharin ($C_7H_5NO_3S$)	-1.07	-1.09	183.18	1.60±0.10	
Caffeine ($C_8H_{10}N_4O_2$)	-0.63	-0.63	194.19	0.52±0.70	
Sulfamethoxazole ($C_{10}H_{11}N_3O_3S$)	0.63	-0.22	253.28	5.81±0.50	
Sucralose ($C_{12}H_{19}Cl_3O_8$)	0.23	0.23	397.63	12.52±0.70	
Trimethoprim ($C_{14}H_{18}N_4O_3$)	-1.33	0.27	290.32	7.04±0.10	
Paracetamol ($C_8H_9NO_2$)	0.48	0.47	151.16	9.86±0.13	
Naproxen ($C_{14}H_{14}O_3$)	2.49	0.73	230.26	4.84±0.30	
Ibuprofen ($C_{13}H_{18}O_2$)	2.81	0.94	206.28	4.41±0.10	
Benzotriazole ($C_6H_5N_3$)	1.44	1.42	119.12	8.38±0.10	
TCEP ($C_6H_{12}Cl_3O_4P$)	1.47	1.47	285.49	NA	
Diclofenac ($C_{14}H_{11}Cl_2NO_2$)	3.66	1.77	296.15	4.18±0.10	

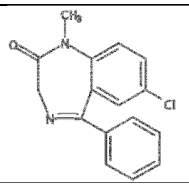
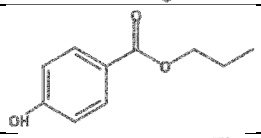
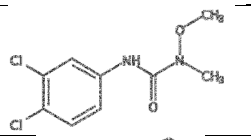
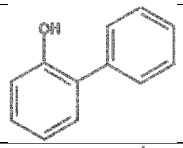
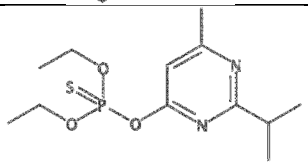
Carbamazepine ($C_{15}H_{12}N_2O$)	1.89	1.89	236.27	13.94±0.20	
Gemfibrozil ($C_{15}H_{22}O_3$)	3.86	2.07	250.33	4.75±0.45	
Verapamil ($C_{27}H_{38}N_2O_4$)	0.98	2.08	454.60	8.97±0.50	
Amitriptyline ($C_{20}H_{23}N$)	1.35	2.28	277.40	9.18±0.28	
Diuron ($C_9H_{10}Cl_2N_2O$)	2.68	2.68	233.09	13.55±0.70	
Benzophenone ($C_{13}H_{10}O$)	3.21	3.21	182.22	NA	
Clozapine ($C_{18}H_{19}ClN_4$)	0.96	3.23	326.82	7.33±0.20	
Bisphenol A ($C_{15}H_{16}O_2$)	3.64	3.64	228.29	10.29±0.10	
Oxybenzone ($C_{14}H_{12}O_3$)	3.99	3.89	228.24	7.56±0.35	
Triclosan ($C_{12}H_7Cl_3O_2$)	5.34	5.28	289.54	7.80±0.35	
Triclocarban ($C_{13}H_9Cl_3N_2O$)	6.07	6.07	315.58	12.77±0.70	

NA: not available.

(B) 20 compounds that were not detectable in primary sludge.

Compounds	Log D at pH=5	Log D at pH=7	MW (g/mol)	pKa	Molecular structure
Acesulfame ($C_4H_5NO_4S$)	-2.88	-2.88	163.15	-0.28±0.40 (-16.62±0.40)	

Cyclamate **(C_6 H_{13} N O_3 S)**	-1.93	-2.46	179.24	-8.66±0.27	
Ketoprofen **(C_{16} H_{14} O_3)**	2.07	0.19	254.28	4.23±0.10	
Meprobamate **(C_9 H_{18} N_2 O_4)**	0.70	0.70	218.25	13.09±0.50 (-1.09±0.70)	
Primidone **(C_{12} H_{14} N_2 O_2)**	0.83	0.83	218.25	1.07±0.40	
PFOS **(C_8 H F_{17} O_3 S)**	1.01	1.01	500.13	-3.27±0.50	
Triamterene **(C_{12} H_{11} N_7)**	-0.34	1.03	253.26	6.28 ± 0.10	
Carazolol **(C_{18} H_{22} N_2 O_2)**	0.54	1.12		13.94±0.20 (9.54±0.30)	
Dilantin **(C_{15} H_{12} N_2 O_2)**	1.42	1.41	252.27	8.28±0.10 (-2.81±0.40)	
Hydroxyzine **(C_{21} H_{27} Cl N_2 O_2)**	0.64	2.15	374.90	14.41±0.10 (6.62±0.10)	
Simazine **(C_7 H_{12} Cl N_5)**	2.28	2.28	201.66	2.71±0.10	
Omeprazole **(C_{17} H_{19} N_3 O_3 S)**	2.18	2.35	345.42	8.78±0.10 (4.72±0.40)	
Atrazine **(C_8 H_{14} Cl N_5)**	2.64	2.64	215.68	2.27±0.10	
PFOA **(C_8 H F_{15} O_2)**	2.77	2.69	414.07	0.50±0.10	

Diazepam **(C_{16} H_{13} Cl N_2 O)**	2.79	2.8	284.74	3.40±0.10	
Propylparaben **(C_{10} H_{12} O_3)**	2.90	2.88	180.20	8.23±0.15	
Linuron **(C_9 H_{10} Cl_2 N_2 O_2)**	3.12	3.12	249.09	12.13±0.70 (-1.04±0.50)	
Phenylphenol **(C_{12} H_{10} O)**	3.29	3.29	170.21	10.00±0.10	
Diazinon **(C_{12} H_{21} N_2 O_3 P S)**	3.77	3.77	304.35	1.21±0.30	
Nonylphenol **(C_{15} H_{24} O)**	6.14	6.14	220.35	10.15±0.15