Electronic Supplementary Information for:

TITLE: Differential biotransformation of micropollutants in conventional activated sludge and up-flow anaerobic sludge blanket processes

AUTHORS: M Martin[a,#], Jingyi Wu[a,#], Stephanie L. Rich[a], Ruth E. Richardson[a], Damian E. Helbling[a,*]

AFFILIATIONS:

[a] School of Civil and Environmental Engineering, Cornell University, Ithaca, NY, 14853, USA

[#] Both authors contributed equally

***** Corresponding author**:** Damian E. Helbling, School of Civil and Environmental Engineering, Cornell University, 220 Hollister Hall, Ithaca, NY, 14853, USA. Email: damian.helbling@cornell.edu. Tel: +1 607 255 5146. Fax: +1 607 255 9004.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

Methods

Micropollutant standards and reagents

Table S1: List of 175 MPs with CAS numbers, chemical formulas, adducts, exact masses, retention times, and diagnostic fragments.

Micropollutant	CAS Number	Chemical Formula	Adduct	Exact Mass (m/z)	RT (min)	Diagnostic Fragment (m/z)
10,11-Dihydrocarbamazepine	3564-73-6	C15H14N2O	$[M+H]^+$	239.1179	6.7	194.10
2-(Methylthio)benzothiazole	615-22-5	C8H7NS2	$[M+H]^+$	182.0092	8.5	135.01
2,2,4-Trimethyl-1,2-dihydroquinoline	147-47-7	C12H15N	$[M+H]^+$	174.1277	6.9	107.07
2,2'-Dithiobis(benzothiazole)	120-78-5	C14H8N2S4	$[M+H]^+$	332.9642	13.9	109.01
2,4-D	94-75-7	C8H6Cl2O3	$[M-H]^-$	218.9621	7.7	160.96
2,6-Dimethoxyphenol	91-10-1	C8H10O3	$[M+H]^+$	155.0708	4.7	95.05
2-Aminobenzothiazole	136-95-8	C7H6N2S	$[M+H]^+$	151.0324	2.7	109.01
2-Ethyl-2-phenylmalonamide	7206-76-0	C11H14N2O2	$[M+H]^+$	207.1134	3.1	119.09
2-Mercaptobenzothiazole	149-30-4	C7H5NS2	$[M+H]^+$	167.9936	5.6	135.01
Abacavir	136470-78-5	C14H18N6O	$[M+H]^+$	287.1620	3.1	191.10
Acebutolol	37517-30-9	C18H28N2O4	$[M+H]^+$	337.2122	4.0	319.20
Acesulfame	33665-90-6	C4H5NO4S	$[M-H]^-$	161.9856	1.5	82.03
Acetaminophen	103-90-2	C8H9NO2	$[M+H]^+$	152.0706	2.1	110.06
Acetazolamide	59-66-5	C4H6N4O3S2	$[M+H]^+$	222.9954	2.2	181.97
Adenosine	58-61-7	C10H13N5O4	$[M+H]^+$	268.1040	1.3	136.06
Adrenalone	99-45-6	C9H11NO3	$[M+H]^+$	182.0812	1.1	146.06
Adrenosterone	382-45-6	C19H24O3	$[M+H]^+$	301.1803	6.2	257.15
Alachlor	15972-60-8	C14H20ClNO2	$[M+H]^+$	270.1255	10.1	162.13
Alachlor OA	171262-17-2	C14H19NO4	$[M-H]^-$	264.1241	6.1	160.11
Albuterol	18559-94-9	C13H21NO3	$[M+H]^+$	240.1594	2.0	148.08
Allopurinol	315-30-0	C5H4N4O	$[M+H]^+$	137.0463	1.3	90.95
Amisulpride	71675-85-9	C17H27N3O4S	$[M+H]^+$	370.1795	3.0	242.05
Amitriptyline	50-48-6	C20H23N	$[M+H]^+$	278.1903	7.3	91.05
Amphetamine	300-62-9	C9H13N	$[M+H]^+$	131.1121	3.0	91.05
Ampicillin	69-53-4	C16H19N3O4S	$[M+H]^+$	350.1169	4.6	192.05
Arecoline	63-75-2	C8H13NO2	$[M+H]^+$	156.1019	1.1	113.06
Atenolol	29122-68-7	C14H22N2O3	$[M+H]^+$	267.1703	2.0	190.09
Atenolol Acid	56392-14-4	C14H21NO4	$[M+H]^+$	268.1543	3.0	191.07
Atomoxetine	83015-26-3	C17H21NO	$[M+H]^+$	256.1696	6.6	224.08
Atorvastatin	134523-00-5	C33H35FN2O5	$[M+H]^+$	559.2603	10.7	440.22

Atrazine	1912-24-9	C8H14ClN5	$[M+H]^+$	216.1011	6.9	174.05
Atrazine-2-hydroxy	2163-68-0	C8H15N5O	$[M+H]^+$	198.1349	3.5	156.09
Atrazine-desethyl	6190-65-4	C6H10ClN5	$[M+H]^+$	188.0697	4.6	146.02
Atropine	55-48-1	C17H23NO3	$[M+H]^+$	290.1751	3.5	260.16
Baclofen	1134-47-0	C10H12ClNO2	$[M+H]^+$	214.0635	3.3	151.03
Bentazone	25057-89-0	C10H12N2O3S	$[M-H]^-$	239.0496	6.3	175.09
Benzophenone	119-61-9	C13H10O	$[M+H]^+$	183.0810	8.7	105.03
Benzothiazole	95-16-9	C7H5NS	$[M+H]^+$	136.0216	5.4	109.01
Benzotriazole	95-14-7	C6H5N3	$[M+H]^+$	120.0556	3.6	92.05
Benzoylecgonine	519-09-5	C16H19NO4	$[M+H]^+$	290.1387	3.7	168.10
Bupropion	34911-55-2	C13H18ClNO	$[M+H]^+$	240.1156	4.8	166.04
Butalbital	77-26-9	C11H16N2O3	$[M-H]^-$	223.1083	5.8	136.37
Caffeine	58-08-2	C8H10N4O2	$[M+H]^+$	195.0877	3.2	138.07
Candesartan	139481-59-7	C24H20N6O3	$[M+H]^+$	441.1670	7.8	263.13
Carbamazepine	298-46-4	C15H12N2O	$[M+H]^+$	237.1022	6.4	194.10
Carbamazepine-10,11-epoxide	36507-30-9	C15H12N2O2	$[M+H]^+$	253.0972	5.1	180.08
Carbendazim	10605-21-7	C9H9N3O2	$[M+H]^+$	192.0768	2.8	160.05
Carisoprodol	78-44-4	C12H24N2O4	$[M+H]^+$	261.1816	7.3	158.12
Celecoxib	169590-42-5	C17H14F3N3O2S	$[M+H]^+$	382.0837	10.5	362.08
Cetirizine	83881-51-0	C21H25ClN2O3	$[M+H]^+$	389.1627	7.8	201.05
Chlorpheniramine	132-22-9	C16H19ClN2	$[M+H]^+$	275.1309	4.8	230.07
Cimetidine	51481-61-9	C10H16N6S	$[M+H]^+$	253.1236	2.1	159.07
Ciprofloxacin	85721-33-1	C17H18FN3O3	$[M+H]^+$	332.1405	3.5	288.15
Citalopram	59729-33-8	C20H21FN2O	$[M+H]^+$	325.1711	5.5	262.10
Citric acid	77-92-9	C6H8O7	$[M-H]^-$	191.0186	1.2	87.92
Clarithromycin	81103-11-9	C38H69NO13	$[M+H]^+$	748.4842	8.3	590.39
Climbazole	38083-17-9	C15H17ClN2O2	$[M+H]^+$	293.1057	6.6	197.07
Clindamycin	18323-44-9	C18H33ClN2O5S	$[M+H]^+$	425.1872	5.6	126.13
Codeine	76-57-3	C18H21NO3	$[M+H]^+$	300.1594	2.2	243.10
Corticosterone	50-22-6	C21H30O4	$[M+H]^+$	347.2217	7.6	121.06
Cotinine	486-56-6	C10H12N2O	$[M+H]^+$	177.1022	1.2	146.06
Coumarin	91-64-5	C9H6O2	$[M+H]^+$	147.0441	4.7	91.05
DEET	134-62-3	C12H17NO	$[M+H]^+$	192.1383	7.1	119.05
Desmethylvenlafaxine	93413-62-8	C16H25NO2	$[M+H]^+$	264.1958	3.9	201.13
Dexamethasone	50-02-2	C22H29FO5	$[M+H]^+$	393.2072	7.6	237.13
Dextromethorphan	125-71-3	C18H25NO	$[M+H]^+$	272.2009	5.5	215.14
Diclofenac	15307-86-5	C14H11Cl2NO2	$[M+H]^+$	296.0240	11.1	215.05
Diethyl phthalate	84-66-2	C12H14O4	$[M+H]^+$	223.0965	7.4	149.02
Dimethyl phthalate	131-11-3	C10H10O4	$[M+H]^+$	195.0652	5.3	149.02

Diphenhydramine	58-73-1	C17H21NO	$[M+H]^+$	256.1701	5.6	167.09
Efavirenz	154598-52-4	C14H9ClF3NO2	$[M+H]^+$	316.0352	11.2	244.01
Emtricitabine	143491-57-0	C8H10FN3O3S	$[M+H]^+$	248.0500	2.0	130.04
Estrone	53-16-7	C18H22O2	$[M+H]^+$	271.1698	8.7	157.06
Ethyl Butylacetylaminopropionate	52304-36-6	C11H21NO3	$[M+H]^+$	216.1594	6.3	188.10
Famciclovir	104227-87-4	C14H19N5O4	$[M+H]^+$	322.1510	3.3	202.11
Famotidine	76824-35-6	C8H15N7O2S3	$[M+H]^+$	338.0527	2.1	189.03
Fenofibric Acid	42017-89-0	C17H15ClO4	$[M+H]^+$	319.0732	10.9	233.04
Fexofenadine	83799-24-0	C32H39NO4	$[M+H]^+$	502.2958	6.9	466.27
Fluconazole	86386-73-4	C13H12F2N6O	$[M+H]^+$	307.1113	4.3	220.07
Flucytosine	2022-85-7	C4H4FN3O	$[M+H]^+$	130.0411	2.0	71.06
Fluoxetine	54910-89-3	C17H18F3NO	$[M+H]^+$	310.1413	7.9	265.16
Fluridone	59756-60-4	C19H14F3NO	$[M+H]^+$	330.1100	8.0	310.10
Furosemide	54-31-9	C12H11ClN2O5S	$[M-H]^-$	328.9999	5.5	204.98
Gabapentin	60142-96-3	C9H17NO2	$[M+H]^+$	172.1332	2.9	137.10
Gabapentin-lactam	64744-50-9	C9H15NO	$[M+H]^+$	154.1227	3.0	137.10
Gemfibrozil	25812-30-0	C15H22O3	$[M+H]^+$	251.1641	13.0	83.09
Hexamethylphosphoramide	680-31-9	C6H18N3OP	$[M+H]^+$	180.1260	4.3	135.07
Hydrochlorothiazide	58-93-5	C7H8ClN3O4S2	$[M-H]^-$	295.9572	2.2	204.98
Hydrocodone	125-29-1	C18H21NO3	$[M+H]^+$	300.1599	2.3	199.08
Hydrocortisone	50-23-7	C21H30O5	$[M+H]^+$	363.2171	6.6	121.06
Ibuprofen	15687-27-1	C13H18O2	$[M+Na]^+$	229.1199	11.5	151.04
Iodocarb	55406-53-6	C8H12INO2	$[M+H]^+$	281.9958	7.0	164.92
Iohexol	66108-95-0	C19H26I3N3O9	$[M+H]^+$	821.8876	1.6	803.88
Iopromide	73334-07-3	C18H24I3N3O8	$[M+H]^+$	791.8770	2.3	572.90
Irbesartan	138402-11-6	C25H28N6O	$[M+H]^+$	429.2397	7.5	386.22
Irgarol	28159-98-0	C11H19N5S	$[M+H]^+$	254.1434	7.4	198.08
Isophorone Diisocyanate	4098-71-9	C12H18N2O2	$[M+K]^+$	261.0995	6.7	204.96
Ketamine	6740-88-1	C13H16ClNO	$[M+H]^+$	238.0998	3.6	179.06
Ketoprofen	22071-15-4	C16H14O3	$[M+H]^+$	255.1016	8.1	209.10
Lamotrigine	84057-84-1	C9H7Cl2N5	$[M+H]^+$	256.0151	4.4	210.98
Levamisole	14769-73-4	C11H12N2S	$[M+H]^+$	205.0794	2.5	178.07
Levetiracetam	102767-28-2	C8H14N2O2	$[M+H]^+$	171.1123	2.6	126.09
Levofloxacin	100986-85-4	C18H20FN3O4	$[M+H]^+$	362.1511	3.6	261.10
Lidocaine	137-58-6	C14H22N2O	$[M+H]^+$	235.1805	3.4	86.10
Losartan	114798-26-4	C22H23ClN6O	$[M+H]^+$	423.1695	7.5	235.10
Mabuterol	56341-08-3	C13H18ClF3N2O	$[M+H]^+$	311.1138	4.4	237.04
Mecoprop	93-65-2	C10H11ClO3	$[M-H]^-$	213.0324	9.3	141.01
Melamine	108-78-1	C3H6N6	$[M+H]^+$	127.0727	1.1	85.05

Meprobamate	57-53-4	C9H18N2O4	$[M+H]^+$	219.1345	5.2	203.14
Metalaxyl	57837-19-1	C15H21NO4	$[M+H]^+$	280.1543	7.2	160.11
Metaxalone	1665-48-1	C12H15NO3	$[M+H]^+$	222.1125	6.7	133.10
Metformin	657-24-9	C4H11N5	$[M+H]^+$	130.1087	1.1	71.06
Methadone	76-99-3	C21H27NO	$[M+H]^+$	310.2165	7.0	265.16
Methocarbamol	532-03-6	C11H15NO5	$[M+H]^+$	242.1028	4.5	163.08
Metolachlor	51218-45-2	C15H22ClNO2	$[M+H]^+$	284.1412	10.1	111.04
Metolachlor ESA	171118-09-5	C15H23NO5S	$[M+H]^+$	330.1370	6.5	298.11
Metolachlor OA	152019-73-3	C15H21NO4	$[M-H]^-$	278.1398	7.6	158.10
Metoprolol	51384-51-1	C15H25NO3	$[M+H]^+$	268.1907	4.0	159.08
Metronidazole	443-48-1	C6H9N3O3	$[M+H]^+$	172.0717	2.0	128.05
Morphine	57-27-2	C17H19NO3	$[M+H]^+$	286.1438	1.4	201.09
N,N-Didesmethylvenlafaxine	93413-77-5	C15H23NO2	$[M+H]^+$	250.1802	5.2	147.08
N4-Acetylsulfamethoxazole	21312-10-7	C12H13N3O4S	$[M+H]^+$	296.0700	4.5	198.02
Nadolol	42200-33-9	C17H27NO4	$[M+H]^+$	310.2013	3.3	254.14
Naproxen	22204-53-1	C14H14O3	$[M+H]^+$	231.1016	8.6	185.10
Nicotine	54-11-5	C10H14N2	$[M+H]^+$	163.1230	1.1	102.97
Norfloxacin	70458-96-7	C16H18FN3O3	$[M+H]^+$	320.1405	3.4	276.15
Ofloxacin	82419-36-1	C18H20FN3O4	$[M+H]^+$	362.1511	3.3	318.16
Oxazepam	604-75-1	C15H11ClN2O2	$[M+H]^+$	287.0558	7.5	241.05
Oxcarbazepine	28721-07-5	C15H12N2O2	$[M+H]^+$	253.0972	5.1	180.08
Oxybenzone	131-57-7	C14H12O3	$[M+H]^+$	229.0864	10.4	151.04
Paraxanthine	611-59-6	C7H8N4O2	$[M+H]^+$	181.0726	2.9	124.05
Penciclovir	39809-25-1	C10H15N5O3	$[M+H]^+$	254.1248	1.3	152.06
Pentobarbital	57-33-0	C11H18N2O3	$[M+H]^+$	227.1396	2.7	86.06
Pentoxifylline	6493-05-6	C13H18N4O3	$[M+H]^+$	279.1457	4.5	181.07
Perfluorobutanoic Acid (PFBA)	375-22-4	C4HF7O2	$[M-H]^-$	212.9792	4.3	168.99
Perfluorooctanoic Acid (PFOA)	335-67-1	C8HF15O2	$[M-H]^-$	412.9664	11.0	168.99
Phenobarbital	50-06-6	C12H12N2O3	$[M-H]^-$	231.0770	5.0	160.08
Phenytoin	57-41-0	C15H12N2O2	$[M+H]^+$	253.0977	6.2	182.10
Primidone	125-33-7	C12H14N2O2	$[M+H]^+$	219.1128	4.4	91.05
Progesterone	57-83-0	C21H30O2	$[M+H]^+$	315.2324	11.1	97.06
Prometon	1610-18-0	C10H19N5O	$[M+H]^+$	226.1662	5.5	142.07
Propazine	139-40-2	C9H16ClN5	$[M+H]^+$	230.1167	8.3	146.02
Propranolol	525-66-6	C16H21NO2	$[M+H]^+$	260.1650	5.5	183.08
Pseudoephedrine	90-82-4	C10H15NO	$[M+H]^+$	166.1229	2.5	148.11
rac threo-Dihydrobupropion	92264-82-9	C13H20ClNO	$[M+H]^+$	242.1306	5.0	162.06
Ranitidine	66357-35-5	C13H22N4O3S	$[M+H]^+$	315.1485	2.0	176.05
Ritalinic Acid	19395-41-6	C13H17NO2	$[M+H]^+$	220.1332	3.8	174.13

Saccharin	81-07-2	C7H5NO3S	$[M-H]^-$	181.9917	2.3	61.97
Serotonin	50-67-9	C10H12N2O	$[M+H]^+$	177.1022	1.1	146.06
Siduron	1982-49-6	C14H20N2O	$[M+H]^+$	233.1654	8.5	137.07
Simazine	122-34-9	C7H12ClN5	$[M+H]^+$	202.0854	5.7	132.03
Sitagliptin	486460-32-6	C16H15F6N5O	$[M+H]^+$	408.1254	4.3	235.08
Sotalol	3930-20-9	C12H20N2O3S	$[M+H]^+$	273.1267	1.8	213.07
Sucralose	56038-13-2	C12H19Cl3O8	$[M+FA-H]^-$	441.0128	3.6	278.15
Sulfadimethoxine	122-11-2	C12H14N4O4S	$[M+H]^+$	311.0809	4.7	156.08
Sulfamethazine	57-68-1	C12H14N4O2S	$[M+H]^+$	279.0910	3.0	204.04
Sulfamethoxazole	723-46-6	C10H11N3O3S	$[M+H]^+$	254.0594	3.8	156.01
Sulfathiazole	72-14-0	C9H9N3O2S2	$[M+H]^+$	256.0209	2.4	108.04
Temazepam	846-50-4	C16H13ClN2O2	$[M+H]^+$	301.0744	7.8	255.07
Testosterone	58-22-0	C19H28O2	$[M+H]^+$	289.2162	9.1	253.20
Theophylline	58-55-9	C7H8N4O2	$[M+H]^+$	181.0726	2.9	124.05
Thiabendazole	148-79-8	C10H7N3S	$[M+H]^+$	202.0433	3.3	175.03
Tramadol	123154-38-1	C16H25NO2	$[M+H]^+$	264.1958	3.9	201.13
Triamterene	396-01-0	C12H11N7	$[M+H]^+$	254.1154	3.8	237.09
Tributyl phosphate	126-73-8	C12H27O4P	$[M+H]^+$	267.1725	12.6	155.05
Triclosan	3380-34-5	C12H7Cl3O2	$[M-H]^-$	286.9439	13.1	165.89
Triethyl phosphate	78-40-0	C6H15O4P	$[M+H]^+$	183.0781	5.1	98.98
Trimethoprim	738-70-5	C14H18N4O3	$[M+H]^+$	291.1452	3.0	245.10
Triphenyl phosphate	115-86-6	C18H15O4P	$[M+H]^+$	327.0781	11.5	327.08
Tris(1,3-dichloro-2-propyl)phosphate (TDCPP)	13674-87-8	C9H15Cl6O4P	$[M+H]^+$	428.8917	11.5	98.98
Tris(2-chloroethyl) phosphate	115-96-8	C6H12Cl3O4P	$[M+H]^+$	284.9612	6.0	160.98
Valsartan	137862-53-4	C24H29N5O3	$[M+H]^+$	436.2343	9.4	235.10
Venlafaxine	93413-69-5	C17H27NO2	$[M+H]^+$	278.2115	5.1	58.07
Verapamil	52-53-9	C27H38N2O4	$[M+H]^+$	455.2910	6.0	303.21
Warfarin	81-81-2	C19H16O4	$[M+H]^+$	309.1121	9.0	251.07

Table S2: List of the 51 isotope labeled internal standards (ILISs).

Internal Standard	CAS Number	Chemical Formula	RT (min)	Adduct	Extracted Mass (m/z)	Reference MP(s)
17-beta-estradiol-d5	221093-45-4	C18H19O2D5	1.0	$[M+H]^+$	278.2162	n/a
2-methyl-3-isothiazolinone-d3	n/a	C4D3H2NOS	1.5	$[M+H]^+$	119.0353	Arecoline, Flucytosine, Melamine
Iodocarb-d9	1246815-08-6	C8H3D9INO2	7.0	$[M+H]^+$	291.0550	Iodocarb, Candesartan
Acetaminophen-d4	64315-36-2	C8D4H5NO2	2.1	$[M+H]^+$	156.0963	2-Aminobenzothiazole, Acetaminophen, Cimetidine, Famotidine, Hydrochlorothiazide, Levamisole
Allopurinol-d2	916979-34-5	C5H2D2N4O	1.3	$[M+H]^+$	139.0583	Cotinine, Adrenalone, Allopurinol, Nicotine, Metformin, Penciclovir
Atenolol-d7	1202864-50-3	C14D7H15N2O3	2.0	$[M+H]^+$	274.2148	Atenolol, Metronidazole, Pentobarbital
Atrazine-d5	163165-75-1	C8H9D5Cl1N5	6.9	$[M+H]^+$	221.1330	2,2,4-Trimethyl-1,2-dihydroquinoline, Atomoxetine, Atrazine-2-hydroxy, Atrazine-desethyl, Climbazole, Metaxalone, Methadone, Simazine
Azoxystrobin-d4	1346606-39-0	C22H13D4N3O5	8.3	$[M+H]^+$	408.1492	Clarithromycin, Corticosterone, Oxazepam, Propazine, Testosterone
Bisphenol A-d16	96210-87-6	C15D16O2	11.7	$[M+H]^+$	245.2227	n/a
Caffeine-13C3	78072-66-9	[13]C3C5H10N4O2	3.2	$[M+H]^+$	198.0977	Caffeine, Levofloxacin, Paraxanthine
Carbamazepine-13C6	n/a	[13]C6C9H12N2O	6.3	$[M+H]^+$	243.1224	10,11-Dihydrocarbamazepine, Carbamazepine, Carbamazepine-10,11-epoxide, DEET, Ethyl Butylacetylaminopropionate, Metolachlor-ESA, Oxcarbazepine
Carbaryl-d7	362049-56-7	C12H4D7NO2	6.2	$[M+H]^+$	209.1302	Hydrocortisone, Prometon
Carbofuran-d3	1007459-98-4	C12H12D3NO3	5.8	$[M+H]^+$	225.1313	2-Mercaptobenzothiazole, Adrenosterone, Dexamethasone, Estrone, Ketoprofen, Pentoxifylline, Phenytoin
Celecoxib-d4	544686-20-6	C17H10D4F3N3O2S	10.5	$[M+H]^+$	386.1083	Celecoxib
Cimetidine-d3	1185237-29-9	C10D3H13N6S	2.1	$[M+H]^+$	256.1418	n/a
Ciprofloxacin-d8	1216659-54-9	C17D8H10FN3O3	3.5	$[M+H]^+$	340.1907	Ciprofloxacin
Citalopram-d6	1246819-94-2	C20D6H15FN2O	5.5	$[M+H]^+$	331.2087	Benzothiazole, Bupropion, Citalopram, Coumarin, Diphenhydramine,
Dextromethorphan-d3	524713-56-2	C18D3H22NO	5.5	$[M+H]^+$	275.2197	Propranolol, Dextromethorphan, Triethyl phosphate
Diazinon-d10	100155-47-3	C12D10H11N2O3PS	7.8	$[M+H]^+$	315.1711	n/a
Diclofenac-13C6	15307-79-6	[13]C6C8H11Cl2NO2	11.1	$[M+H]^+$	302.0441	Diclofenac, Fenofibric acid, Progesterone
Diltiazem-d4	*112259-40-2*	C22D4H22N2O4S	6.1	$[M+H]^+$	419.1937	Clindamycin, , Verapamil

Dimethoate-d6	1219794-81-6	C5H6D6NO3PS2	4.2	$[M+H]^+$	236.0446	2,6-Dimethoxyphenol, Acebutolol, Fluconazole, Hexamethylphosphoramide, Lamotrigine, Mabuterol, Methocarbamol, Metoprolol, N4-Acetylsulfamethoxazole, Primidone, Sitagliptin
Erythromycin-13C,d3	114-07-8	[13]CC36D3H64NO13	6.8	$[M+H]^+$	738.4907	n/a
Estrone-d2	350820-16-5	C18H20D2O2	8.7	$[M+H]^+$	273.1818	Irgarol, Warfarin
Fexofenadine-d6	548783-71-7	C32H33D6NO4	6.9	$[M+H]^+$	508.3328	, Fexofenadine
Fluoxetine-d5	1173020-43-3	C17D5H13F3NO	7.9	$[M+H]^+$	315.1727	Cetirizine, Fluoxetine, Fluridone
Gemfibrozil-d6	1184986-45-5	C15H16D6O3	13.0	$[M+H]^+$	257.2018	Gemfibrozil
Ibuprofen-d3	121662-14-4	C13D3H15O2	11.5	$[M+H]^+$	232.1387	Atorvastatin, Ibuprofen, Tributyl phosphate
Imidacloprid-d4	1015855-75-0	C9D4H6Cl1N5O2	3.8	$[M+H]^+$	260.0852	NA
Iopromide-d3	1189947-73-6	C18D3H21I3N3O8	2.3	$[M+H]^+$	794.8959	2-(Methylthio)benzothiazole, 2-Ethyl-2-phenylmalonamide, Iopromide, Levetiracetam, Pseudoephedrine
Isoproturon-d6	217487-17-7	C12H12D6N2O	7.2	$[M+H]^+$	213.1869	Amitriptyline, Benzophenone, Carisoprodol, Diethyl phthalate, Dimethyl phthalate, Irbesartan, Isophorone Diisocyanate, Losartan, Metalaxyl, Temazepam, Valsartan
Mecoprop-d3	352431-15-3	C10H8D3ClO3	9.3	$[M-H]^-$	216.0501	2,4-D, Acesulfame, Bentazone, Butalbital, Mecoprop, , Metolachlor OA
Metformin-d6	1185166-01-1	C4D6H5N5	1.1	$[M+H]^+$	136.1464	n/a
Metoprolol Acid-d5	1215404-47-9	C14H16D5NO4	3.0	$[M+H]^+$	273.1863	Amphetamine, Atenolol acid, Acetazolamide, Albuterol, Amisulpride, Carbendazim, Codeine, , Gabapentin, Gabapentin-lactam, Norfloxacin, Ofloxacin
Morphine-d3	67293-88-3	C17D3H16NO3	1.4	$[M+H]^+$	289.1626	Adenosine, Emtricitabine, Hydrocodone, Iohexol, Morphine, Serotonin, Sotalol
Naproxen-methoxy-d3	958293-79-3	C14D3H11O3	8.6	$[M+H]^+$	234.1204	Metolachlor, Naproxen, Siduron
Oxybenzone-d3	131-57-7	C14H9D3O3	10.4	$[M+H]^+$	232.1048	, Oxybenzone
Pirimicarb-d6	1015854-66-6	C11D6H12N4O2	3.8	$[M+H]^+$	245.1879	Tramadol
rac-Efavirenz-d4	1246812-58-7	C14H5D4ClF3NO2	11.1	$[M+H]^+$	320.0597	Efavirenz, Triphenyl phosphate
Ranitidine-d6	1185238-09-8	C13H16D6N4O3S	2.0	$[M+H]^+$	321.1862	Ranitidine
Sertraline-d3	1217741-83-7	C17D3H14Cl2N	8.3	$[M+H]^+$	309.0999	n/a
Sucralose-d6	1459161-55-7	C12H13D6Cl3O8	3.6	$[M-H]^-$	447.0499	Alachlor OA, Citric acid, Furosemide, Phenobarbital, Saccharin, Sucralose
Sulfadimethoxine-d6	73068-02-7	C12D6H8N4O4S	4.7	$[M+H]^+$	317.1185	Ampicillin, Sulfadimethoxine, Sulfamethazine, Sulfamethoxazole, Sulfathiazole
Sulfamethoxazole-(phenyl-13C6)	1196157-90-0	[13]C6C4H11N3O3S	3.8	$[M+H]^+$	260.0795	n/a
13C8 – PFOA	n/a	[13]C8HF15O2	11.0	$[M-H]^-$	420.9921	PFBA, PFOA

13C8 – PFOS	n/a	[13]C8HF17O3S	12.0	$[M-H]^-$	506.9559	n/a
Thiabendazole-d4	1190007-20-5	C10H3D4N3S	3.3	$[M+H]^+$	206.0685	Atropine, Baclofen, Benzotriazole, Benzoylecgonine, Famciclovir, Ketamine, Lidocaine, Nadolol, Ritalinic acid, Thiabendazole, Triamterene
Triclosan-d3	1020719-98-5	C12H4D3Cl3O2	13.1	$[M-H]^-$	289.9627	Triclosan
Trimethoprim-d9	1189460-62-5	C14D9H9N4O3	2.9	$[M+H]^+$	300.2016	Abacavir, Trimethoprim
Tris(2-chloroethyl)phosphate-d12	1276500-47-0	C6D12Cl3O4P	6.0	$[M+H]^+$	297.0365	, TDCPP, Tris(2-chloroethyl) phosphate
Venlafaxine-d6	1062606-12-5	C17D6H21NO2	5.1	$[M+H]^+$	284.2491	Chlorpheniramine, Meprobamate, N,N-Didesmethylvenlafaxine, O-Desmethylvenlafaxine, rac threo-Dihydrobupropion, Venlafaxine

n/a = information not available

Table S3: List of 24 MPs used in batch experiments with CAS numbers, chemical formulas, adducts, exact masses, retention times, and diagnostic fragments.

Micropollutant	pK_a	Species at neutral pH	logD	$logK_{oc}$	K_d
Acetaminophen	9.46	neutral	0.75	1.32	7.31
Caffeine	n/a	neutral	-0.7	0.98	0.07
Adrenosterone	n/a	neutral	2.81	2.1	44.06
N4-acetylsulfamethoxazole	5.88	negative	-0.3	1.71	17.95
Theophylline	11.44	neutral	-0.73	1	3.5
Serotonin	9.31	positive	-1.01	1.19	5.42
Ethyl_butylacetylaminopropionate	n/a	neutral	0.94	1.65	15.63
Amphetamine	10.01	positive	-0.55	1.88	26.55
Gabapentin	9.91	neutral	1.09	-0.47	0.12
Benzoylecgonine	9.54	neutral	-0.38	-0.7	0.07
Diphenhydramine	8.87	positive	2.39	2.58	133.07
Bupropion	8.22	positive	2.89	3.21	567.63
Sotalol	9.43	positive	-2.41	0.74	1.92
DEET	n/a	neutral	2.59	1.86	25.36
Ketoprofen	3.88	negative	0.69	2.08	42.08
2,4-D	2.81	negative	-0.87	1.77	20.61
Mecoprop	3.47	negative	-0.23	1.98	33.42
Tramadol	9.23	positive	0.85	1.96	31.92
Methocarbamol	13.36	neutral	0.43	0.88	2.66
Lamotrigine	5.87	neutral	2.11	2.18	52.97
Losartan	8.30	neutral	5.27	3.2	554.71
Bentazone	2.03	negative	0.01	2.11	45.09
Ritalinic_Acid	10.08	neutral	-0.11	-0.48	0.12
Acesulfame	3.02	negative	-1.43	0.35	0.78

Field sampling campaign

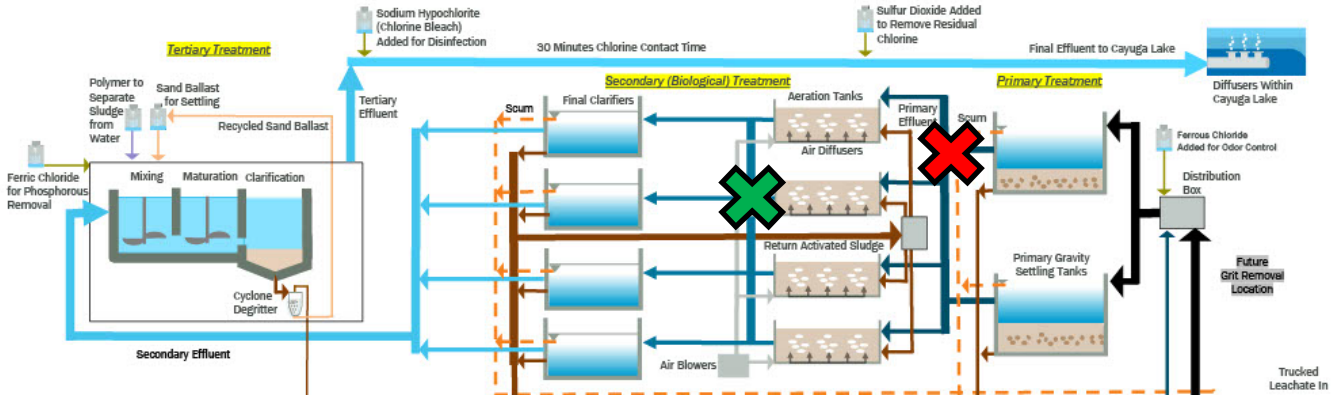

Figure S1: Process flow diagram of the studied WWTP along with sampling locations depicted with a red (CAS_inf) and green (CAS_eff) X symbol. We note that the influent samples for the CAS process (CAS_inf) were collected after primary settling and before mixing with the return activated sludge. (source: https://www.cityofithaca.org/687/Plant-Schematic)

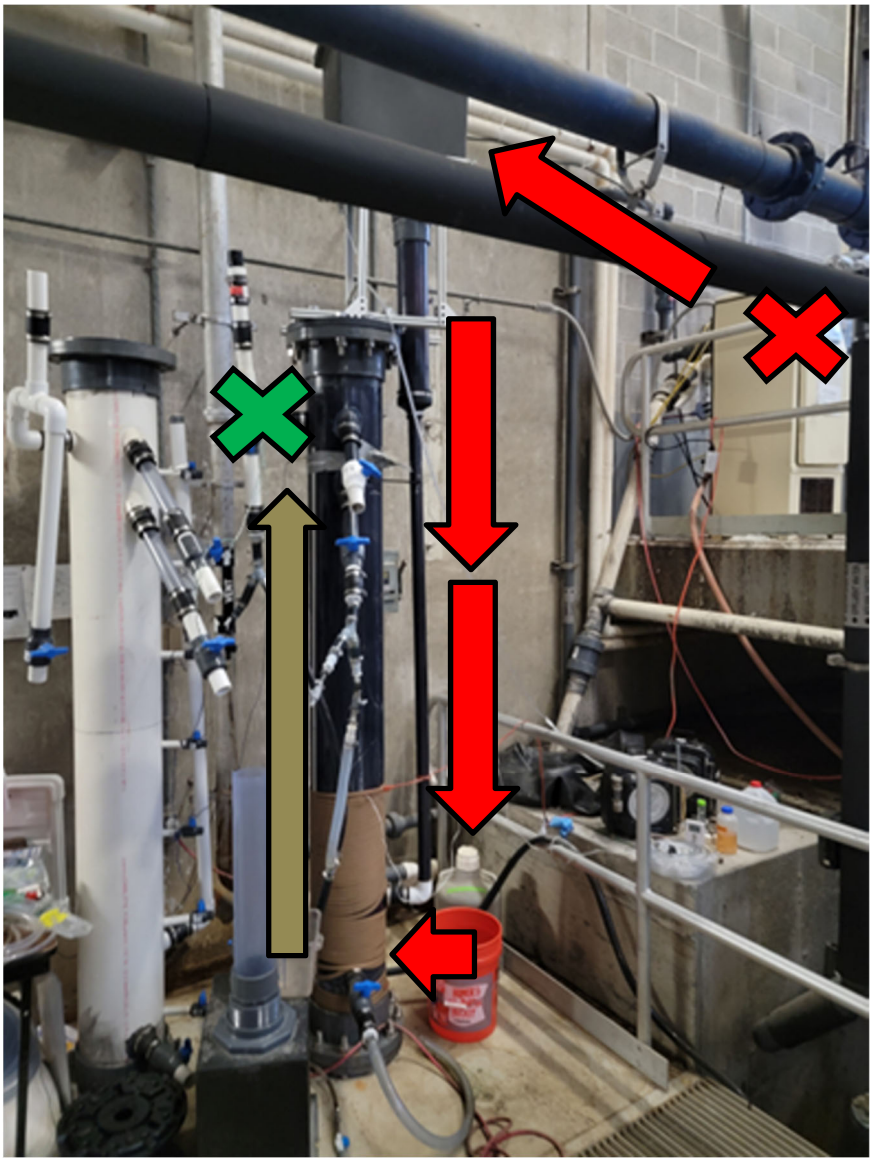

Figure S2: Process flow diagram of the studied UASB along with sampling locations depicted with a red (UASB_inf) and green (UASB_eff) X symbol. We note that the influent samples for the UASB process (UASB_inf) were collected from the outlet of a peristaltic pump that feeds untreated wastewater (after bar screening) to the UASB.

Table S4: WWTP operational parameters measured during the sampling period.

	UASB Inf	UASB Eff	CAS Inf	CAS Eff
pH	7.57	7.23	7.48	7.19
T (°C)	21.1	22.4	21.2	22
HRT	9.5 hours		8 hours	
	UASB - top	**UASB - bottom**	**CAS Center**	
Sludge/Granule TSS (mg/mL)[1]	7.2	36.4	1.2	

[1]sludge was collected from the top and bottom of the UASB for TSS analysis.

Preparation of wastewater samples

The self-packed mixed bed cartridges contained three layers separated by polyethylene frits. The bottom layer consisted of 200 mg Envi-CARB (Supelclean) media. The middle layer was 350 mg of a 1:1:1.5 (by mass) mixture of Strata X-AW (Phenomenex), Strata X-CW (Phenomenex), and Isolute ENV+ (Biotage), respectively. The final layer was 200 mg of Oasis HLB (Waters) media. The cartridges were conditioned before sample loading by passing a mixture of 5 mL methanol and 10 mL nanopure water through each cartridge. The sample loading rate was controlled at approximately 1-3 drops per second. The cartridges were eluted using 6 mL of 50:50 v/v ethyl acetate/methanol with 0.5% ammonia, 3 mL of 50:50 v/v ethyl acetate/methanol with 1.7% formic acid, and 2 mL of pure methanol. The extracts were evaporated under a stream of high-purity nitrogen to 100 μL and reconstituted to 1 mL using nanopure water. The extracted samples were filtered (regenerated cellulose, 0.45 μm, Thermo Scientific) and stored at -20 ˚C and in the dark until analysis. We also prepared a 9-point calibration curve by spiking the mixture of the 175 MPs into 1 L of nanopure water to generate standards at concentrations of 0, 1, 5, 25, 50, 100, 250, 500, and 750 ng L^{-1}. The calibration standards were likewise spiked with 20 μL of the ILIS mixture and loaded onto the mixed-bed SPE cartridges and eluted as described in the preceding.

Sample Analysis

Briefly, samples were measured using reversed-phase liquid chromatography (Ultimate 3000, Thermo Scientific) coupled to high-resolution quadrupole-orbitrap mass spectrometry (QExactive, Thermo Scientific) with 30 µL injections of samples stored at 4 °C during the analysis. Samples were separated using a mobile phase gradient of LC-MS grade water (OmniSolv, 58201, solvent A) and methanol (OmniSolv, 58215, solvent B) – both containing 0.1% (v/v) formic acid – over an XBridge C18 column (Waters, 186003021, particle size: 3.5 µm, flow rate: 0.2 mL/min, gradient properties: 0 – 5 min: 5% B, 5 – 21 min: 5% B – 95% B (linear increase), 21 – 25 min: 95% B, 25 – 30 min: 5% B). We performed full-scan MS acquisitions (100-1000 m/z, resolution 140,000) in electrospray ionization positive-negative switch mode. Data dependent MS2 spectra were acquired at the exact masses and retention times of all target MPs and ILISs with additional MS2 spectra collected for the TopN MS features if the inclusion list was not triggered. For absolute quantification of target analytes, we used ILIS normalized peak areas obtained with Xcalibur Quanbrowser (Thermo Scientific, Version 4.0.27.19) and a calibration series (concentration range: 0-750 µg/L after passing through SPE) with 1/x least-squares regression.

Quality Control

Table S5: List of MPs with R^2, LOQ, and number of detections in *CAS_inf*, *CAS_eff*, *UASB_inf*, *UASB_eff* samples.

Micropollutant	R^2	LOQ (ng/L)	N UASB_inf	N UASB_eff	N CAS_inf	N CAS_eff
10,11-dihydrocarbamazepine	0.9978	1	0	0	0	0
2-Aminobenzothiazole	0.9864	1	0	0	0	0
2-ethyl-2-phenyl_malonamide	0.9819	25	9	0	6	0
2-Mercaptobenzothiazole	0.0076	DNM	DNM	DNM	DNM	DNM
2-Methylthiobenzothiazole	0.1013	DNM	DNM	DNM	DNM	DNM
2,2,4-Trimethyl-1,2-Dihydr	1.0000	500	0	0	0	0
2,2_-Dithiobis(benzothiazole)	0.0145	DNM	DNM	DNM	DNM	DNM
2,4-D	0.9990	1	9	8	9	9
2,6-dimethoxyphenol	0.0128	DNM	DNM	DNM	DNM	DNM
Abacavir	0.9934	25	0	0	0	0
Acebutolol	0.9786	50	0	0	0	0
Acesulfame	0.8882	1	9	9	9	9
Acetaminophen	0.9822	1	9	9	9	9
Acetazolamide	0.9986	25	0	0	0	0
Acetochlor_Alachlor	0.9759	5	0	0	0	0
Adenosine	0.0115	DNM	DNM	DNM	DNM	DNM
Adrenalone	0.0201	DNM	DNM	DNM	DNM	DNM
Adrenosterone	0.9916	1	9	9	9	9
Alachlor-OXA	0.9304	1	2	0	2	8
Albuterol	0.9943	1	0	0	0	0
Allopurinol	0.0190	DNM	DNM	DNM	DNM	DNM
Amisulpride	0.9815	25	0	0	0	0
Amitriptyline	0.9387	50	0	0	0	0
Amphetamine	0.9950	1	8	9	9	6
Ampicillin	1.0000	500	0	0	0	0
Arecoline	0.9027	5	9	8	5	1
Atenolol	0.9955	1	9	9	9	9
Atenolol_Acid	0.9969	1	9	9	9	9
Atomoxetine	0.8148	5	0	0	0	0
Atorvastatin	0.9571	25	0	0	0	0
Atrazine	0.9892	1	0	1	0	7
Atrazine-2-hydroxy	0.7951	DNM	DNM	DNM	DNM	DNM
Atrazine-desethyl	0.8799	250	0	0	0	0
Atropine	0.9506	50	4	8	0	7
Baclofen	0.9499	50	0	0	0	0
Bentazone	0.9749	1	9	9	9	9
Benzophenone	0.0015	DNM	DNM	DNM	DNM	DNM
Benzothiazole	0.0237	DNM	DNM	DNM	DNM	DNM
Benzotriazole	0.9556	100	9	9	9	9
Benzotriazole_methyl-1H	0.9903	1	9	9	9	9
Benzoylecgonine	0.9924	50	9	9	9	9
Bupropion	0.9954	25	6	9	9	9
Butalbital	0.9703	1	2	0	3	1
Caffeine	0.8979	50	9	9	9	8
Candesartan	0.9960	5	0	0	0	0
Carbamazepine	0.1958	DNM	DNM	DNM	DNM	DNM
Carbamazepine-10,11-epoxide	0.9950	1	5	9	9	9
Carbendazim	0.9980	25	0	9	0	9

Carisoprodol	0.9994	1	1	1	0	0
Celecoxib	0.9924	5	0	0	0	0
Cetirizine	0.8999	1	9	0	9	9
Chlorpheniramine	0.9958	100	0	0	0	0
Cimetidine	0.8669	250	0	0	0	0
Ciprofloxacin	1.0000	250	0	0	0	0
Citalopram	0.9978	25	0	0	4	9
Citric_Acid	0.0007	DNM	DNM	DNM	DNM	DNM
Clarithromycin	0.9882	25	0	0	0	5
Climbazole	0.7393	DNM	DNM	DNM	DNM	DNM
Clindamycin	0.8677	25	0	0	0	9
Codeine	0.9914	25	2	9	0	6
Corticosterone	0.9988	1	9	3	9	0
Cotinine	0.9771	1	9	4	9	4
Coumarin	0.7260	DNM	DNM	DNM	DNM	DNM
DEET	0.9779	1	9	9	9	9
Desmethylvenlafaxine	0.9919	25	9	9	9	9
Dexamethasone	0.9392	1	0	0	0	0
Dextromethorphan	0.9989	25	0	0	1	8
Diclofenac	0.9972	5	0	0	0	0
Diethyl_phthalate	0.0218	DNM	DNM	DNM	DNM	DNM
Dimethyl_phthalate	0.4040	DNM	DNM	DNM	DNM	DNM
Diphenhydramine	0.9249	1	7	3	9	9
Efavirenz	0.9956	25	0	0	0	0
Emtricitabine	0.9501	50	0	9	6	9
Estrone	0.0315	DNM	DNM	DNM	DNM	DNM
Ethyl_butylacetylaminoprop	0.8874	1	9	9	9	9
Famciclovir	1.0000	500	0	0	0	0
Famotidine	1.0000	500	0	0	0	1
Fenofibric_Acid	0.9408	1	9	0	9	8
Fexofenadine	0.9944	1	8	0	9	2
Fluconazole	0.9884	25	7	9	9	9
Flucytosine	0.9731	25	0	8	1	9
Fluoxetine	0.6895	DNM	DNM	DNM	DNM	DNM
Fluridone	0.7890	DNM	DNM	DNM	DNM	DNM
Furosemide	0.9494	5	5	0	9	7
Gabapentin	0.9687	25	9	9	9	9
Gabapentin_lactam	0.9387	100	9	9	9	9
Gemfibrozil	0.4566	DNM	DNM	DNM	DNM	DNM
Hexamethylphosphoramide	0.9975	25	0	0	0	2
Hydrochlorothiazide	0.9903	5	0	0	0	0
Hydrocodone	0.9884	25	3	9	2	6
Hydrocortisone	0.9899	1	1	4	3	3
Ibuprofen_Na	0.9954	50	0	0	0	0
Iodocarb	0.0000	DNM	DNM	DNM	DNM	DNM
Iohexol	0.9468	250	3	9	9	9
Iopromide	0.9725	250	0	0	0	0
Irbesartan	0.9925	1	2	0	9	9
Irgarol	0.9893	1	0	0	0	0
Isophorone_Diisocyanate_K	0.9900	25	0	0	0	0
Ketamine	0.9558	50	0	1	0	9
Ketoprofen	0.9941	1	8	0	9	2
Lamotrigine	0.9930	50	9	9	9	9
Levamisol	0.9950	25	0	0	0	5

Levetiracetam	0.9777	5	9	0	6	0
Levofloxacin	0.9637	50	0	0	0	0
Lidocaine	0.9231	50	9	9	9	9
Losartan	0.9893	5	9	8	9	9
Mabuterol	0.9929	50	0	0	0	0
Mecoprop	0.9989	1	9	9	9	9
Melamine	1.0000	750	0	0	0	0
Meprobamate	0.9757	25	0	0	0	0
Metalaxyl	0.9976	1	9	9	9	9
Metaxalone	0.5730	DNM	DNM	DNM	DNM	DNM
Metformin	0.5952	DNM	DNM	DNM	DNM	DNM
Methadone	0.8458	1	0	0	0	9
Methocarbamol	0.9853	50	8	9	9	9
Metolachlor	0.9659	1	0	0	0	0
Metolachlor-ESA	0.9878	5	0	0	0	0
Metolachlor-OXA	0.9973	1	9	9	9	9
Metoprolol	0.9782	25	9	9	8	9
Metronidazole	0.9883	5	0	0	0	9
Morphine	0.9986	5	1	0	0	0
N,N-didesmethylvenlafaxine	0.9860	5	6	9	5	9
N4-acetylsulfamethoxazole	0.9913	25	9	0	9	9
Nadolol	0.9706	25	0	1	0	5
Naproxen	0.1369	DNM	DNM	DNM	DNM	DNM
Nicotine	0.9276	1	9	4	9	4
Norfloxacin	0.9509	250	0	0	0	0
Ofloxacin	0.9485	50	0	0	0	0
Oxazepam	0.9694	5	0	0	0	4
Oxcarbazepine	0.9950	1	5	9	9	9
Oxybenzone	0.8724	1	0	0	0	0
Theophylline	0.9705	5	9	9	9	1
Penciclovir	0.8086	DNM	DNM	DNM	DNM	DNM
Pentobarbital	0.0433	DNM	DNM	DNM	DNM	DNM
Pentoxyfylline	0.9905	25	0	0	2	0
Perfluorooctanoic_Acid	0.9921	1	9	9	9	9
PFBA	0.9948	1	0	0	0	0
Phenobarbital	0.9438	5	2	0	3	3
Phenytoin	0.0050	DNM	DNM	DNM	DNM	DNM
Primidone	0.9937	50	3	9	0	9
Progesterone	0.0014	DNM	DNM	DNM	DNM	DNM
Prometon	0.9926	1	0	0	0	0
Propazine	0.8721	1	0	0	0	3
Propranolol	0.0093	DNM	DNM	DNM	DNM	DNM
Pseudoephedrine	0.9567	1	9	0	9	0
rac-threo-Dihydrobupropion	0.9964	5	0	0	0	0
Ranitidine	1.0000	500	0	0	0	0
Ritalinic_Acid	0.9803	50	9	9	8	9
Saccharin	0.9349	1	8	0	9	8
Serotonin	0.9925	1	9	9	9	9
Siduron	0.7962	DNM	DNM	DNM	DNM	DNM
Simazine	0.0356	DNM	DNM	DNM	DNM	DNM
Sitagliptin	0.9251	250	0	0	0	0
Sotalol	0.9968	5	5	8	8	9
Sucralose_FA	0.4073	DNM	DNM	DNM	DNM	DNM
Sulfadimethoxine	0.9774	100	0	0	0	0

Sulfamethazine	0.9100	250	0	0	0	0
Sulfamethoxazole	0.9754	250	3	2	4	6
Sulfathiazole	0.9672	50	0	0	0	0
TDCPP	0.8421	1	0	0	0	0
Temazepam	0.9909	1	0	1	0	8
Testosterone	0.9944	1	9	9	9	9
Thiabendazole	0.9735	25	0	0	0	0
Tramadol	0.9943	25	9	9	9	9
Triamterene	0.9766	50	0	0	0	0
Tributyl_phosphate	0.8598	1	2	0	7	0
Triclosan	0.0765	DNM	DNM	DNM	DNM	DNM
Triethylphosphate	0.6438	DNM	DNM	DNM	DNM	DNM
Trimethoprim	0.9952	1	4	0	9	1
Triphenyl_phosphate	0.5174	DNM	DNM	DNM	DNM	DNM
Tris(2-chloroethyl)phosphate	0.9429	1	0	0	2	0
Valsartan	0.5874	DNM	DNM	DNM	DNM	DNM
Venlafaxine	0.9909	1	9	9	9	9
Verapamil	0.9933	25	0	0	0	0
Warfarin	0.0234	DNM	DNM	DNM	DNM	DNM

Results and Discussion

Summary data from sampling of full-scale CAS and UASB.

Table S6: List of 88 MPs measured in *CAS_inf* and *UASB_inf* and their average concentration in all samples.

MPs	R^2	LOQ	Average UASB_inf [µg/L]	Average UASB_eff [µg/L]	Average CAS_inf [µg/L]	Average CAS_eff [µg/L]
2,4-D	0.9990	1	308	30	211	134
2-ethyl-2-phenyl_malonamide	0.9819	25	2772	0	717	0
Acesulfame	0.8882	1	17314	11082	16792	1920
Acetaminophen	0.9822	1	111043	18705	60697	2267
Adrenosterone	0.9916	1	2942	332	2295	159
Alachlor-OXA	0.9304	1	1328	0	98	109
Amphetamine	0.9950	1	1601	659	685	69
Arecoline	0.9027	5	298	256	117	277
Atenolol	0.9955	1	1580	968	693	771
Atenolol_Acid	0.9969	1	4603	4052	3106	4340
Atrazine	0.9892	1	0	11	0	18
Atropine	0.9506	50	688	208	0	83
Bentazone	0.9749	1	17	6	3	2
Benzotriazole	0.9556	100	5595	51015	9081	5722
Benzotriazole_methyl-1H	0.9903	1	21616	70399	36431	47196
Benzoylecgonine	0.9924	50	6562	51540	4079	599
Bupropion	0.9954	25	1761	627	2861	3087
Butalbital	0.9703	1	83	0	25	33
Caffeine	0.8979	50	71771	21833	40506	965
Carbamazepine-10,11-epoxide	0.9950	1	258	298	311	268
Carbendazim	0.9980	25	0	163	0	140
Carisoprodol	0.9994	1	41	19	0	0
Cetirizine	0.8999	1	1606	0	975	1840
Citalopram	0.9978	25	0	0	442	345
Clarithromycin	0.9882	25	0	0	0	387
Clindamycin	0.8677	25	0	0	0	637
Codeine	0.9914	25	254	105	0	70
Corticosterone	0.9988	1	1462	1095	805	0
Cotinine	0.9771	1	1186	723	895	122
DEET	0.9779	1	7206	9658	3967	985
Desmethylvenlafaxine	0.9919	25	2080	6339	1758	2662
Dextromethorphan	0.9989	25	0	0	261	271
Diphenhydramine	0.9249	1	1204	108	1725	1835
Emtricitabine	0.9501	50	0	6058	1732	3724

Ethyl_butylacetylaminopropionate	0.8874	1	3544	890	3770	430
Famotidine	1.0000	500	0	0	0	6184
Fenofibric_Acid	0.9408	1	24287	0	24223	42692
Fexofenadine	0.9944	1	4630	0	4848	15658
Fluconazole	0.9884	25	758	338	367	398
Flucytosine	0.9731	25	0	21834	2773	8478
Furosemide	0.9494	5	1398	0	702	329
Gabapentin	0.9687	25	12158	9413	6129	1289
Gabapentin_lactam	0.9387	100	12617	15387	6219	3446
Hexamethylphosphoramide	0.9975	25	0	0	0	29
Hydrocodone	0.9884	25	349	190	265	168
Hydrocortisone	0.9899	1	1179	194	421	169
Iohexol	0.9468	250	54611	95882	82017	58500
Irbesartan	0.9925	1	65	0	75	109
Ketamine	0.9558	50	0	391	0	133
Ketoprofen	0.9941	1	131	0	94	26
Lamotrigine	0.9930	50	817	712	1145	2833
Levamisol	0.9950	25	0	0	0	123
Levetiracetam	0.9777	5	20232	0	9140	0
Lidocaine	0.9231	50	1752	5230	886	1317
Losartan	0.9893	5	423	177	505	359
Mecoprop	0.9989	1	3494	1732	795	1463
Metalaxyl	0.9976	1	226	91	50	69
Methadone	0.8458	1	0	0	0	8
Methocarbamol	0.9853	50	1989	838	1068	1071
Metolachlor-OXA	0.9973	1	79	77	81	53
Metoprolol	0.9782	25	1271	1248	1048	2097
Metronidazole	0.9883	5	0	0	0	195
Morphine	0.9986	5	232	0	0	0
N,N-didesmethylvenlafaxine	0.9860	5	406	115	67	80
N4-acetylsulfamethoxazole	0.9913	25	925	0	823	257
Nadolol	0.9706	25	0	219	0	111
Nicotine	0.9276	1	8976	108	2686	50
Oxazepam	0.9694	5	0	0	0	119
Oxcarbazepine	0.9950	1	258	298	311	268
Paraxanthine_Theophylline	0.9705	5	8713	3116	6600	145
Pentoxyfylline	0.9905	25	0	0	717	0
Perfluorooctanoic_Acid	0.9921	1	428	105	172	114
Phenobarbital	0.9438	5	869	0	283	650
Primidone	0.9937	50	1268	475	0	467
Propazine	0.8721	1	0	0	0	14

Pseudoephedrine	0.9567	1	12284	0	2842	0
Ritalinic_Acid	0.9803	50	1246	6722	911	502
Saccharin	0.9349	1	96225	0	46736	11998
Serotonin	0.9925	1	1298	1581	866	277
Sotalol	0.9968	5	562	377	218	368
Sulfamethoxazole	0.9754	250	3845	5172	3806	4671
Temazepam	0.9909	1	0	26	0	105
Testosterone	0.9944	1	1142	2863	312	283
Tramadol	0.9943	25	1107	995	1138	2021
Tributyl_phosphate	0.8598	1	148	0	1323	0
Trimethoprim	0.9952	1	2335	0	966	637
Tris(2-chloroethyl)phosphate	0.9429	1	0	0	138	0
Venlafaxine	0.9909	1	711	858	704	931

Batch experiments – biotransformation products

Table S7: Analytical information for the 9 detected TPs.

Parent MP	TP	Formula of Neutral Molecule	Exact Mass of [M+H]+ Adduct	Extracted Mass	RT (min)	Fragment (m/z)	Found in UASB _eff?[2]	Found in CAS _eff?
Caffeine	Caf_181	C7H8N4O2	181.0720	181.0791	2.66	124.05 84.96	NO	NO
Diphenhydramine	Dip_181	C13H8O	183.0810	183.0805	8.63	105.03	YES	YES
Diphenhydramine	Dip_288	C17H21NO2	272.1645	272.1643	5.89	NF	NO	NO
Amphetamine	Amp_168	C9H13NO	152.1070	152.1069	1.75	94.06 107.05	NO	NO
N-acetylsulfamethoxazole	N-SMX_254	C10H11N3O3S	254.0594	254.0591	3.65	108.04 156.01	YES	YES
Ethyl-butylacetylamino-propionate	EBP_188	C9H17NO3	188.1281	188.1279	4.50	NF	NO	YES
Adrenosterone	Adr_301	C19H24O3	301.1798	301.1794	6.17	257.15 121.06	NO	NO
Adrenosterone	Adr_331	C20H26O4	331.1904	331.1876	13.92	161.09	NO	NO

[1]NF = no MS2 fragment could be identified; [2]UASB_eff and CAS_eff samples were screened for evidence of peaks at the extracted mass and RT of each TP.