

Supplementary Information

Characterization, source and risk of pharmaceutically active compounds (PhACs) in the snow deposition near Jiaozhou Bay, North China

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S1:Detailed substance information and monitoring parameters

Table 1. Category, compound name, CAS number, molecular formula of all target analytes, and monitoring parameters in liquid chromatography coupled with tandem mass spectrometry.

Substance Information					Monitoring Parameters			
Num	Category	Compound	Molecular formula	CAS number	ESI	Precursor Ion (m/z)	Product Ion 1 (m/z)	Product Ion 2 (m/z)
1	Antibiotics (15 Sulfonamides)	Sulfadiazine	C10H10N4O2S	68-35-9	+	251	156	92
2		Sulfathiazole	C9H9N3O2S2	72-14-0	+	256	156	108
3		Sulfapyridine	C11H11N3O2S	144-83-2	+	250	156	108
4		Sulfamerazine	C11H12N4O2S	127-79-7	+	265	172	156
5		Sulfamethazine	C12H14N4O2S	57-68-1	+	279	186	156
6		sulfamonomethoxine	C11H12N4O3S	1220-83-3	+	281	156	126
7		Sulfamethizole	C9H10N4O2S2	144-82-1	+	271	156	108
8		Sulfameter	C11H12N4O3S	651-06-9	+	281	156	108
9		sulfachloropyridazine	C10H9ClN4O2S	80-32-0	+	285	156	108
10		sulfamethoxypyridazine	C11H12N4O3S	80-35-3	+	281	156	126
11		Sulfadoxine	C12H14N4O4S	2447-57-6	+	311	156	126
12		Sulfadimethoxine	C12H14N4O4S	122-11-2	+	311	218	156
13		Sulfamethoxazole	C10H11N3O3S	723-46-6	+	254	156	108
14		Sulfisoxazole	C11H13N3O3S	127-69-5	+	268	156	113

15		Sulfabenzamide	C13H12N2O3S	127-71-9	+	277	156	108
16	Antibiotics (10 Quinolones)	Enrofloxacin	C19H22FN3O3	93106-60-6	+	360	316	245
17		Norfloxacin	C16H18FN3O3	70458-96-7	+	320	276	233
18		Pefloxacin	C17H20FN3O3	70458-92-3	+	334	316	290
19		Ciprofloxacin	C17H18FN3O3	85721-33-1	+	332	288	245
20		Ofloxacin	C18H20FN3O4	82419-36-1	+	362	318	261
21		Sarafloxacin	C20H17F2N3O3	98105-99-8	+	386	342	299
22		Enoxacin	C15H17FN4O3	74011-58-8	+	321	303	324
23		Lomefloxacin	C17H19F2N3O3	98079-51-7	+	352	308	265
24		Nalidixic acid	C12H12N2O3	389-08-2	+	233	215	187
25		Oxolinic acid	C13H11NO5	14698-29-4	+	262	244	216
26	Antibiotics (5 Macrolide Antibiotics)	Erythromycin	C37H67NO13	114-07-8	+	734	576	158
27		Roxithromycin	C41H76N2O15	80214-83-1	+	837	679	158
28		Josamycin	C42H69NO15	16846-24-5	+	828	174	109
29		Tylosin	C46H77NO17	1401-69-0	+	916	772	174
30		Tilmicosin	C46H80N2O13	108050-54-0	+	869	696	174
31	Antibiotics (15 Cephalosporins)	Cephalexin	C16H17N3O4S	15686-71-2	+	348	174	158
32		Cefapirin	C17H17N3O6S2	21593-23-7	+	424	292	152
33		Cefaclor	C15H14ClN3O4S	53994-73-3	+	368	174	105
34		Cefixime	C16H15N5O7S2	79350-37-1	+	454	285	126

35		Cephradine	C16H19N3O4S	38821-53-3	+	350	176	158
36		Cefpirome	C22H22N6O5S2	84957-29-9	+	515	167	120
37		Cefetamet pivoxyl	C20H25N5O7S2	65243-33-6	+	512	241	126
38		Cefazolin	C14H14N8O4S3	25953-19-9	+	455	323	156
39		Desacetylcefotaxime	C14H15N5O6S2	66340-28-1	+	414	241	125
40		Cefamandole	C18H18N6O5S2	58648-57-0	+	463	347	158
41		Ceftiofur	C19H17N5O7S3	80370-57-6	+	524	241	125
42		Cefotaxime	C16H17N5O7S2	63527-52-6	+	456	167	125
43		Ceftazidime	C22H32N6O12S2	78439-06-2	+	547	468	167
44		Cephalonium	C20H18N4O5S2	5575-21-3	+	459	152	123
45		Cefquinome	C23H24N6O5S2	84957-30-2	+	529	396	134
46	Antibiotics (4 Tetracyclines)	Tetracycline	C22H24N2O8	60-54-8	+	445	427	410
47		Oxytetracycline	C22H24N2O9	79-57-2	+	461	443	426
48		Chlortetracycline	C22H23ClN2O8	57-62-5	+	479	462	444
49		Doxycycline	C22H24N2O8	564-25-0	+	445	428	154
50	10 Imidazoles	Dimetridazole	C5H7N3O2	551-92-8	+	142	96	81
51		Ronidazole	C6H8N4O4	7681-76-7	+	201	140	55
52		5-chloro-1-methyl-4-nitroimidazole	C4H4ClN3O2	4897-25-0	+	162	145	116
53		5-nitrobenzimidazole	C7H5N3O2	94-52-0	+	164	118	91
54		Iprnidazole	C7H11N3O2	14885-29-1	+	170	124	109

55		Albendazole	C12H15N3O2S	54965-21-8	+	266	234	191
56		Albendazole	C12H15N3O3S	54029-12-8	+	282	240	208
57		Flubendazole	C16H12FN3O3	31430-15-6	+	314	282	123
58		Fenbendazole	C15H13N3O2S	43210-67-9	+	300	268	159
59		Oxfendazole	C15H13N3O3S	53716-50-0	+	316	191	159
60	10 NSAIDs	Tenoxicam	C13H11N3O4S2	59804-37-4	+	338	121	78
61		Indoprofen	C17H15NO3	31842-01-0	+	282	236	218
62		Meloxicam	C14H13N3O4S2	71125-38-7	+	352	141	115
63		Flunixin	C14H11F3N2O2	42461-84-7	+	297	279	264
64		Mefenamic acid	C15H15NO2	61-68-7	+	242	224	209
65		Diclofenac	C14H9Cl2NO	15307-86-5	+	296	250	215
66		Piroxicam	C15H13N3O4S	36322-90-4	+	332	164	95
67		Nabumetone	C15H16O2	42924-53-8	+	229	171	128
68		Sulindac	C20H17FO3S	38194-50-2	+	357	340	233
69		Indomethacin	C19H16ClNO4	53-86-1	+	358	139	111
70	5 Hypoglycemic Drugs	Glibenclamide	C23H28ClN3O5S	10238-21-8	+	491	369	169
71		Glimepiride	C24H34N4O5S	93479-97-1	+	491	352	126
72		Glipizide	C21H27N5O4S	29094-61-9	+	446	321	103
73		Repaglinde	C27H36N2O4	135062-02-1	+	453	230	162
74		Tolbutamide	C12H18N2O3S	64-77-7	+	270	155	91

75	20 hormones	Prednisone	C21H26O5	53-03-2	+	359	147	341
76		Cortisone	C21H28O5	53-06-5	+	361	163	121
77		Beclomethasone	C22H29ClO5	4419-39-0	+	409	391	279
78		Flumethasone	C22H28F2O5	2135-17-3	+	411	253	121
79		Methylprednisolone 21-acetate	C24H32O6	53-36-1	+	417	253	161
80		Fludrocortisone 21-acetate	C23H31FO6	514-36-3	+	423	239	343
81		Budesonide	C25H34O6	51372-29-3	+	431	413	147
82		Amcinonide	C28H35FO7	51022-69-6	+	503	339	321
83		Fluticasone	C25H31F3O5S	80474-14-2	+	501	313	293
84		Triamcinolone diacetate	C25H31FO8	67-78-7	+	479	441	147
85		Prednisolone	C21H28O5	50-24-8	+	361	343	147
86		Dexamethasone	C22H29FO5	50-02-2	+	393	373	355
87		Mometason	C27H30Cl2O6	105102-22-5	+	521	503	263
88		Fluocinonide	C26H32F2O7	356-12-7	+	495	337	121
89		Medroxyprogesterone	C24H34O4	71-58-9	+	387	327	249
90		Methyltestosterone	C20H30O2	58-18-4	+	303	109	97
91		Testosterone propionate	C22H32O3	57-85-2	+	345	97	109
92		Chlormadinone acetate	C23H29ClO4	302-22-7	+	405	309	345
93		Boldenone	C19H26O2	846-48-0	+	287	121	135
94		Trenbolone	C18H22O2	10161-33-8	+	271	253	199

95	8 Antipsychotic drugs	midazolam	C18H13ClFN3	59467-70-8	+	326	291	249
96		Alprazolam	C17H13ClN4	28981-97-7	+	309	281	205
97		Clonazepam	C15H10ClN3O3	1622-61-3	+	316	270	214
98		Diazepam	C16H13ClN2O	439-14-5	+	285	193	154
99		Lorazepam	C15H10Cl2N2O2	846-49-1	+	321	275	229
100		Triazolam	C17H12Cl2N4	28911-01-5	+	343	308	239
101		Oxazepam	C15H11ClN2O2	604-75-1	+	287	269	241
102		Nitrazepam	C15H11N3O3	146-22-5	+	282	236	180
103	6 β -Adrenergic Receptors	Ractopamine	C18H23NO3	97825-25-7	+	302	164	107
104		Salbutamol	C13H21NO3	18559-94-9	+	240	222	148
105		Terbutaline	C12H19NO3	23031-25-6	+	226	152	107
106		Cimaterol	C12H17N3O	54239-37-1	+	220	202	160
107		Clenbuterol	C12H18Cl2N2O	37148-27-9	+	277	203	168
108		Tulobuterol	C12H18ClNO	41570-61-0	+	228	154	118
109	Antihypertensive drugs	Propranolol	C16H21NO2	525-66-6	+	260	183	116
110	Antiviral drugs	Amantadine	C10H17N	768-94-5	+	152	135	93
IS 1	Internal standard	Cimaterol-d7	C12H10D7N3O	1228182-44-2	+	227	209	161
IS 2	(IS)	Ractopamine-d6	C18H17D6ClNO3	1276197-17-1	+	308	290	168

IS 3		Roxithromycin-D7	C41H69D7N2O15	2095110-69-1	+	845	686	558
IS 4		Sulfamethoxazole-d4	C10H7D4N3O3S	1020719-86-1	+	258	192	160
IS 5		Norfloxacin-d5	C16H13D5FN3O3	1015856-57-1	+	325	307	281

S2: Study area and physicochemical parameters

Table 2. Sampling station's, locations, silicate , phosphates, nitrites, nitrates, ammonium, total organic carbon (TOC) from each station.

Sampling Station	Latitude, N	Longitude, E	PO ₄ -P (µg/L)	NO ₃ -N (µg/L)	NO ₂ -N (µg/L)	NH ₄ -N (µg/L)	SiO ₃ -Si (µg/L)	TOC (mg/L)
S1	36°09'49"	120°22'03"	216.83	904.96	42.04	402.15	154.66	8.25
S2	36°08'58"	120°20'48"	78.35	495.89	30.76	872.10	70.86	3.77
S3	36°07'37"	120°19'59"	160.19	853.55	29.46	796.49	120.84	6.82
S4	36°06'48"	120°19'58"	24.43	415.58	24.26	1197.30	70.96	2.29
S5	36°05'2"	120°19'02"	105.61	465.14	20.58	1106.42	113.13	2.54
S6	36°03'51"	120°17'48"	50.16	491.86	14.08	1251.23	96.82	2.96
S7	36°03'46"	120°18'51"	31.66	447.93	11.74	937.95	128.09	94.83
S8	36°03'28"	120°20'22"	96.70	580.11	4.20	738.45	147.60	3.43
S9	36°03'08"	120°21'07"	63.88	368.69	17.70	847.57	92.84	3.43
S10	36°03'43"	120°22'49"	114.08	394.84	33.91	914.21	247.12	3.89
S11	36°03'35"	120°25'26"	73.04	619.24	14.57	1002.02	345.22	4.50
S12	36°04'50"	120°27'12"	51.26	374.93	16.13	1164.47	90.32	3.47
S13	36°05'48"	120°30'17"	71.86	716.74	15.14	738.90	130.50	5.85
S14	36°04'14"	120°20'52"	362.59	741.96	4.67	1713.92	270.70	7.15
S15	36°04'37"	120°21'29"	71.49	595.50	18.22	1247.44	69.43	5.47
S16	36°05'20"	120°22'21"	44.15	407.82	15.79	1016.26	119.55	5.36
S17	36°06'56"	120°23'09"	68.74	375.44	6.35	1021.57	128.91	7.22
S18	36°08'24"	120°25'20"	718.66	625.11	41.31	1416.85	343.65	17.18
S19	36°09'52"	120°25'51"	22.83	411.19	22.80	1078.65	83.63	2.17

S3: Occurrence data

Table S3. ^cConcentrations obtained in each sample (ng/L).

Num	Analytes	LOQ	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	Mean Value	Maximum Value	Minimum Value	Frequency of Detection %
1	Chlormadinone acetate	0.17	0.26	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.20	0.44	N.D.	N.D.	N.D.	0.29	N.D.	0.06	0.44	0.00	21.05
2	Trenbolone	0.15	N.D.	N.D.	0.30	N.D.	N.D.	N.D.	N.D.	0.20	N.D.	N.D.	N.D.	N.D.	N.D.	1.56	N.D.	N.D.	N.D.	N.D.	N.D.	0.11	1.56	0.00	15.79
3	Tolbutamide	0.2	0.59	0.57	N.D.	N.D.	N.D.	N.D.	0.74	N.D.	N.D.	N.D.	0.50	N.D.	0.92	N.D.	0.93	N.D.	0.98	0.62	N.D.	0.31	0.98	0.00	42.11
4	Prednisone	0.5	1.19	N.D.	0.87	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.99	N.D.	1.53	N.D.	N.D.	N.D.	N.D.	0.24	1.53	0.00	21.05
5	Methylprednisolone 21-acetate	0.5	N.D.	N.D.	N.D.	N.D.	1.01	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	4.84	N.D.	N.D.	0.82	N.D.	N.D.	N.D.	0.35	4.84	0.00	15.79
6	Fludrocortisone 21-acetate	1.0	N.D.	N.D.	N.D.	N.D.	1.86	N.D.	1.44	11.80	N.D.	N.D.	N.D.	N.D.	N.D.	12.00	1.70	N.D.	5.47	1.32	3.46	2.06	12.00	0.00	42.11
7	Budesonide	0.1	1.00	N.D.	2.57	N.D.	0.12	4.27	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.22	3.27	N.D.	N.D.	N.D.	N.D.	N.D.	0.64	4.27	0.00	31.58
8	Triamcinolone diacetate	2.0	14.30	N.D.	30.50	N.D.	N.D.	90.10	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	25.50	N.D.	N.D.	6.68	N.D.	N.D.	N.D.	8.79	90.10	0.00	26.32
9	Fluocinonide	0.3	1.58	0.45	1.47	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	2.88	N.D.	1.26	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.40	2.88	0.00	26.32
10	Flunixin	0.06	N.D.	0.13	N.D.	N.D.	0.11	N.D.	N.D.	0.12	0.13	N.D.	N.D.	0.11	0.12	N.D.	0.15	0.13	N.D.	0.10	0.16	0.07	0.16	0.00	52.63
11	Piroxicam	0.1	N.D.	N.D.	N.D.	N.D.	0.16	N.D.	N.D.	N.D.	0.11	N.D.	N.D.	N.D.	N.D.	0.24	N.D.	N.D.	N.D.	N.D.	N.D.	0.03	0.24	0.00	15.79
12	Indomethacin	0.5	3.17	N.D.	3.19	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.89	N.D.	0.38	3.19	0.00	15.79
13	Sulfadiazine	0.06	N.D.	N.D.	N.D.	N.D.	0.10	N.D.	N.D.	N.D.	N.D.	0.20	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.16	N.D.	0.03	0.20	0.00	15.79
14	Sulfamerazine	0.03	0.08	N.D.	0.08	N.D.	N.D.	N.D.	N.D.	N.D.	0.07	N.D.	N.D.	N.D.	0.05	0.07	N.D.	N.D.	N.D.	N.D.	N.D.	0.02	0.08	0.00	26.32
15	sulfamonomethoxine	0.2	0.57	0.56	0.56	0.56	0.56	0.55	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.56	0.58	0.56	0.56	0.58	0.55	100.00
16	sulfameter	0.2	0.48	0.49	0.46	0.46	0.46	0.53	0.45	0.45	0.46	0.46	0.47	0.46	0.49	0.68	0.47	0.46	0.47	2.17	0.46	0.57	2.17	0.45	100.00
17	sulfamethoxyppyridazine	0.2	0.45	0.48	0.46	0.46	0.47	0.54	0.45	0.45	0.47	0.47	0.47	0.46	0.48	0.65	0.45	0.46	0.47	0.47	0.46	0.48	0.65	0.45	100.00
18	Sulfamethoxazole	1.0	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	3.95	N.D.	0.21	3.95	0.00	5.26
19	Lorazepam	0.1	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.14	N.D.	N.D.	0.15	N.D.	N.D.	0.17	N.D.	0.02	0.17	0.00	15.79
20	Nitrazepam	0.1	0.22	0.21	0.26	0.21	0.21	0.21	0.22	0.21	0.25	0.28	0.22	0.22	0.22	0.27	0.22	0.21	0.29	0.35	0.21	0.24	0.35	0.21	100.00
21	Dimetridazole	0.5	N.D.	0.63	N.D.	N.D.	0.75	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.07	0.75	0.00	10.53
22	Ronidazole	2.0	5.34	13.80	12.80	26.90	23.70	30.90	21.10	9.55	18.00	15.70	14.70	23.90	12.10	8.60	13.40	21.00	31.00	11.60	22.70	17.73	31.00	5.34	100.00
23	5-chloto-1-methyl-4-nitroimidazole	0.5	2.19	1.92	1.36	0.90	1.34	0.94	1.25	1.23	0.80	0.81	0.68	1.11	0.57	0.87	1.47	0.51	1.23	0.68	0.83	1.09	2.19	0.51	100.00
24	5-nitrobenzimidazole	0.1	3.86	1.33	1.81	0.52	0.56	0.29	0.25	0.19	1.97	1.32	0.17	3.26	0.39	0.12	0.67	0.85	0.55	0.12	1.42	1.03	3.86	0.12	100.00
25	Salbutamol	0.1	2.03	2.30	0.28	3.49	2.69	2.64	1.97	4.62	2.75	2.88	2.43	2.96	0.36	1.60	4.92	5.92	3.11	0.10	6.85	2.84	6.85	0.10	100.00
26	Norfloxacin	1.6	N.D.	N.D.	2.87	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	11.50	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.76	11.50	0.00	10.53
27	Pefloxacin	1.2	N.D.	N.D.	1.94	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.00	N.D.	N.D.	N.D.	N.D.	6.43	0.44	6.43	0.00	10.53
28	Oxolinic acid	0.1	N.D.	N.D.	N.D.	N.D.	0.17	N.D.	N.D.	0.16	0.17	0.17	0.17	N.D.	N.D.	0.15	0.15	0.26	0.22	N.D.	0.27	0.10	0.27	0.00	52.63
29	Roxithromycin	0.1	N.D.	0.16	0.26	0.14	0.60	0.12	0.11	0.11	0.13	0.19	0.13	0.11	0.10	0.31	0.13	0.14	0.21	0.23	0.19	0.18	0.60	0.00	94.74
30	Josamycin	0.05	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.11	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.01	0.11	0.00	5.26
31	Tilmicosin	1.0	2.64	N.D.	1.71	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	2.02	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.34	2.64	0.00	15.79
32	Cefixime	1.3	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	2.13	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.12	2.13	0.00	5.26
33	Cefetamet pivoxyl	0.5	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	0.85	N.D.	N.D.	N.D.	N.D.	N.D.	0.04	0.85	0.00	5.26
34	Desacetylcefotaxime	1.6	63.60	51.90	101.00	59.70	34.60	32.50	22.90	48.50	36.80	48.80	24.00	24.20	46.50	69.60	67.20	30.60	16.20	92.80	27.80	47.33	101.00	16.20	100.00
35	Cefamandole	1.1	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	5.42	N.D.	N.D.	N.D.	N.D.	N.D.	0.29	5.42	0.00	5.26
36	Ceftiofur	0.7	1.04	N.D.	1.50	2.05	1.26	1.26	1.36	2.63	1.25	1.55	N.D.	N.D.	2.14	2.08	2.26	1.23	N.D.	5.61	N.D.	1.43	5.61	0.00	73.68
37	Cephalonium	1.8	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	7.70	N.D.	0.41	7.70	0.00	5.26
38	Tetracycline	2.3	126.00	N.D.	105.00	N.D.	27.60	18.60	N.D.	7.07	5.15	567.00	N.D.	15.60	4.99	1500.00	N.D.	7.41	N.D.	5.98	N.D.	125.81	1500.00	0.00	63.16

^cMean of three determinations;

N.D.: not detected (<LOQ).

S4: Statistical Analysis

Table S4: Spearman correlation coefficients

compound	Chlormadinone acetate	Trenbolone	Tolbutamide	Prednisone	Methylprednisolone 21-acetate	Fludrocortisone 21-acetate	Budesonide	Triamcinolone diacetate	Fluocinonide	Flunixin	Piroxicam	Indomethacin	Sulfadiazine	Sulfamerazine	Sulfamonomethoxine	Sulfamethoxyypyridazine	Sulfamethoxazole	Lorazepam	Nitrazepam	Dimetridazole	Ronidazole	5-chloro-1-methyl-4-nitroimidazole	5-nitrobenzimidazole	Salbutamol	Norfl oxacin	Pefloxacin	Oxolinic acid	Roxithromycin	Josamycin	Tilmicosin	Cefixime	Cefamandole	Cefepime	Ceftiofur	Cephazolin	Tetracycline	PO ₄ ³⁻	NO ₃ ⁻	NO ₂ ⁻	NH ₄ ⁺	SiO ₂	TOC	Total detections				
Chlormadinone acetate	1.000																																														
Trenbolone	0.227	1.000																																													
Tolbutamide	0.268	-0.350	1.000																																												
Prednisone	0.297	0.074	0.435	1.000																																											
Methylprednisolone 21-acetate	-0.221	-0.186	0.157	0.141	1.000																																										
Fludrocortisone 21-acetate	0.140	0.383	0.128	-0.175	0.121	1.000																																									
Budesonide	0.453	0.418	-0.161	0.382	-0.064	-0.052	1.000																																								
Triamcinolone diacetate	0.203	0.382	-0.164	0.235	0.102	-0.233	0.712	1.000																																							
Fluocinonide	-0.002	0.068	-0.135	0.273	-0.254	-0.479	0.129	0.205	1.000																																						
Flunixin	-0.188	-0.206	-0.018	0.077	0.087	0.113	-0.387	-0.570	-0.239	1.000																																					
Piroxicam	0.227	0.293	-0.350	-0.221	0.207	0.332	0.323	0.027	-0.254	0.037	1.000																																				
Indomethacin	0.439	0.248	0.118	0.472	-0.186	-0.194	0.351	0.427	0.457	-0.293	-0.186	1.000																																			
Sulfadiazine	0.147	-0.186	-0.088	-0.221	0.165	0.060	-0.087	-0.254	0.176	-0.116	0.165	0.165	1.000																																		
Sulfamerazine	0.518	0.456	-0.049	0.542	-0.254	-0.184	0.619	0.461	0.296	-0.180	0.356	0.531	-0.254	1.000																																	
Sulfamonomethoxine	0.590	-0.062	0.355	0.256	-0.062	0.058	-0.181	-0.175	0.233	0.000	-0.062	0.640	0.330	0.249	1.000																																
Sulfameter	0.661	-0.062	0.385	0.214	0.014	-0.065	0.427	0.370	-0.047	-0.127	0.060	0.224	0.055	0.206	0.173	1.000																															
Sulfamethoxyypyridazine	0.275	0.006	-0.076	-0.312	-0.039	-0.102	0.366	0.205	-0.129	-0.139	0.397	-0.232	0.203	0.086	-0.307	0.642	1.000																														
Sulfamethoxazole	0.483	-0.102	0.240	-0.121	-0.102	0.096	-0.156	-0.139	-0.139	0.000	-0.102	0.474	0.542	-0.139	0.610	0.404	0.111	1.000																													
Lorazepam	0.186	-0.186	0.291	0.184	0.165	0.077	-0.286	-0.254	0.004	0.260	-0.186	0.202	0.248	-0.254	0.372	0.241	-0.201	0.610	1.000																												
Nitrazepam	0.422	0.171	0.339	0.141	-0.137	0.084	0.023	0.088	0.218	-0.394	0.115	0.385	0.311	0.364	0.405	0.285	0.184	0.404	0.298	1.000																											
Dimetridazole	-0.175	-0.148	-0.048	-0.175	0.345	0.051	0.052	-0.202	0.085	0.241	0.345	-0.148	0.293	-0.202	-0.049	0.050	0.283	-0.081	-0.148	-0.391	1.000																										
Ronidazole	-0.662	-0.501	-0.176	-0.492	0.032	-0.084	-0.251	-0.217	-0.218	-0.060	-0.077	-0.493	-0.040	-0.552	-0.557	-0.303	0.075	-0.258	-0.112	-0.279	0.105	1.000																									
5-chloro-1-methyl-4-nitroimidazole	-0.172	0.158	0.194	0.352	0.107	0.179	0.192	0.142	0.394	-0.107	-0.044	0.258	-0.169	0.095	0.041	-0.097	-0.371	-0.280	0.019	-0.147	0.402	-0.061	1.000																								

[illegible]

S5: Risk assessment

Table S5. Maximum measured concentration (MECs), acute toxicity data EC₅₀ of the studied compounds on the aquatic organisms, and predicted no effect concentrations (PNECs) and the estimated risk quotients (RQs).

PhACs	Taxonomic group	EC ₅₀ (mg/L)	PNEC(ng/L)	MECs(ng/L)	RQs	Reference
Sulfadiazine	Fish	1516.102	1516102	0.20	0.0000	[a]
	Daphnia	174.400	174400		0.0000	[1]
	Algae	0.103	103		0.0019	[2]
Sulfamethoxazole	Fish	520.500	520500	3.95	0.0000	[a]
	Daphnia	25.2	252000		0.0000	[a]
	Algae	0.03	30		0.13	[a]
Sulfamerazine	Algae	11.9	11900	0.08	0.0000	[3]
	Plant	0.68	680		0.0002	[4]
Sulfamethoxypyridazine	Algae	3.82	3820	0.65	0.02	[3]
	Fish	589.3	589300		0.0000	[5]
Sulfamonomethoxine	Algae	8.56	8560	0.58	0.0000	[a]
	Daphnia	48	48000		0.0000	[6]
	Fish	>1000			0.0000	[6]
Norfloxacin	Plants	0.913	913	11.50	0.0126	[7]
	Algae	51.18	51180		0.0002	[7]
Ronidazole	Algae	1.080	1080	31.00	0.0287	[a]
	Daphnia	19.445	19445		0.0002	[a]
	Fish	242.023	242023		0.0000	[a]
Oxolinic acid	Fish	4466.764	4466764	0.27	0.0000	[a]
	Daphnia	4.600	4600		0.0000	[8]
	Algae	16.000	16000		0.0000	[9]
Roxithromycin	Plants	>1	1000	0.6	0.0006	[7]
	Invertebrates	7.1	7100		0.0000	[7]
Tetracycline	Invertebrates	0.0417	41.7	1500.00	35.971	[a]
	Fish		260000			
	Algae	0.09	90		16.667	[a]
Indomethacin	Fish	42.9352	42935	3.19	0.0000	[a]
Prednisone	Fish	110.916	110916	1.53	0.0000	[a]
	Daphnia	0.23	230		0.0067	[a]

Note: a = predicted value by ECOSAR

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