Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting Information

Persistent, Mobile, and Toxic Plastic Additives in Canada: Properties and Prioritization

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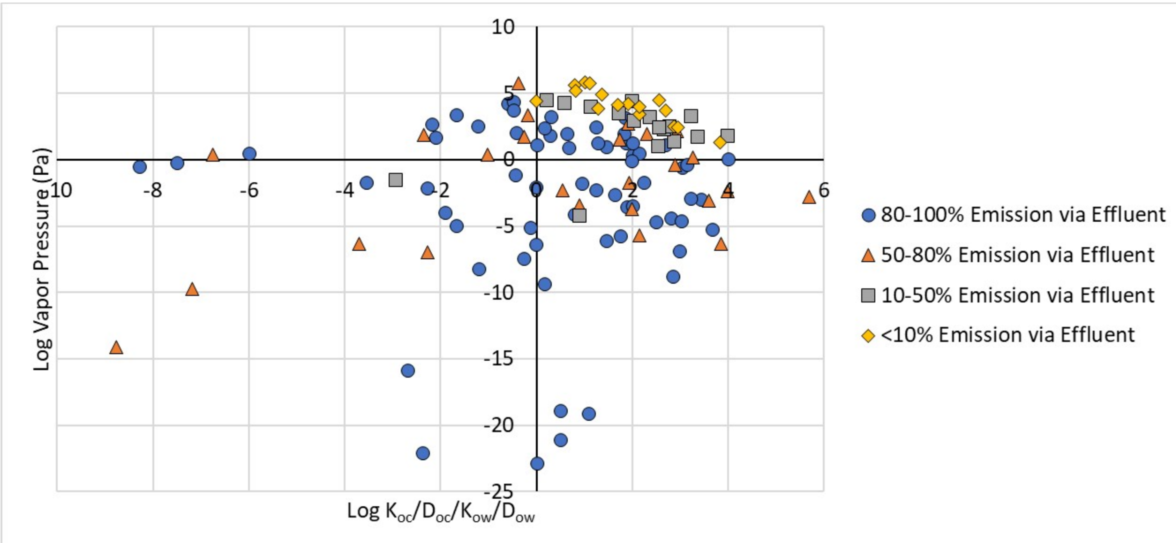

Figure S1. Log $K_{oc}/D_{oc}/K_{ow}/D_{ow}$ versus log vapour pressure (Pa) graph of 124 PMT plastic additives plotted according to their predicted percent emission via effluent in a WWTP simulation.

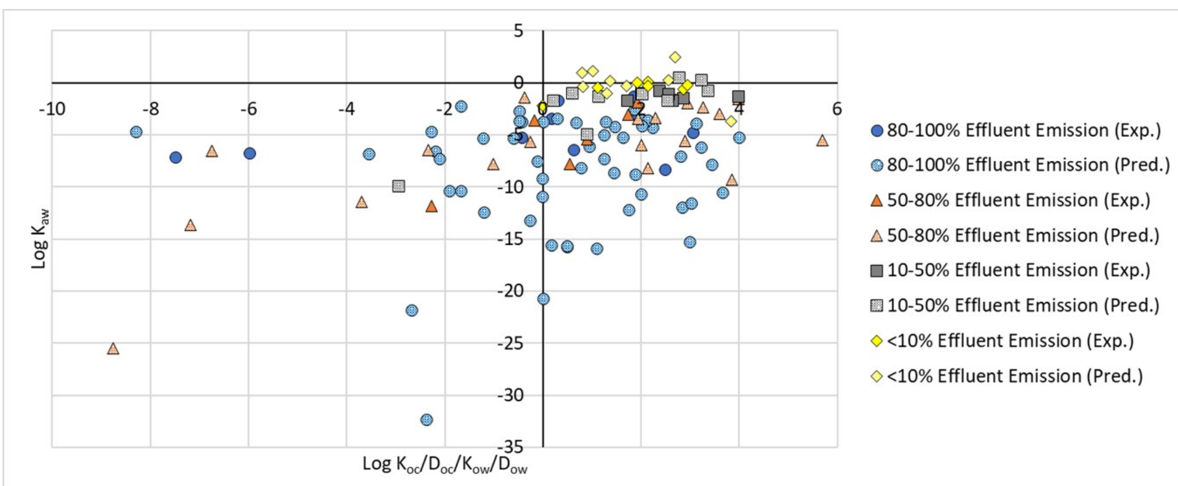

Figure S2. Log Koc/Doc/Kow/Dow versus log Kaw for the 124 PMT plastic additives, plotted according to their predicted percent emission via effluent, and whether both property values were experimental data (Exp.) or at least one value was predicted data (Pred.).

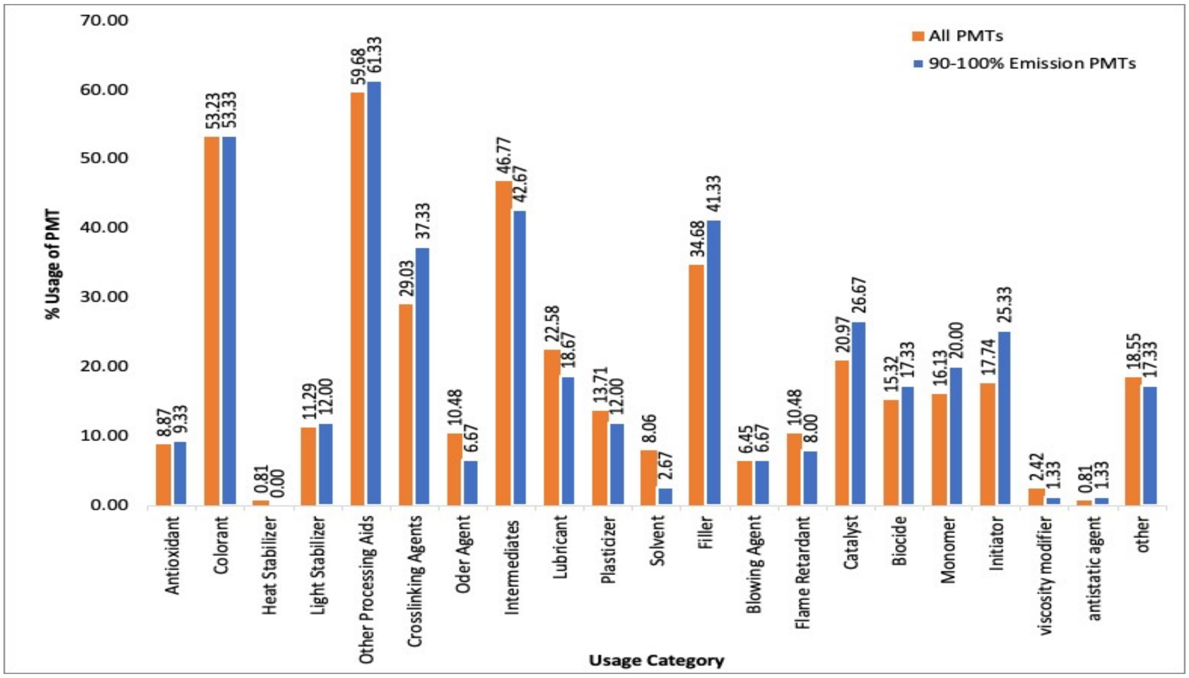

Figure S3. Bar chart of the use functions of the 124 PMT plastic additives. The orange bars indicate the percent of all PMTs and their uses by category and the blue bars indicate the percent of all the PMTs with a 80-100% emission via effluent for the given category.

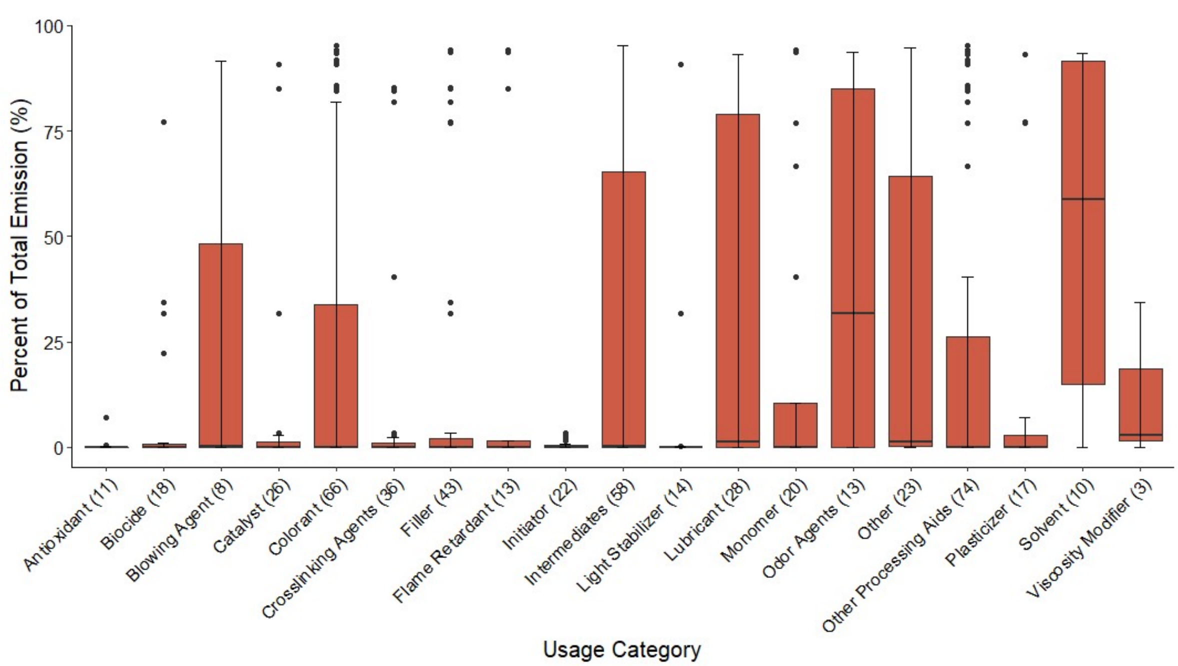

Figure S4: The distribution of air emission (as a percentage of total emission) of 124 PMT plastic additives, based on their use category.

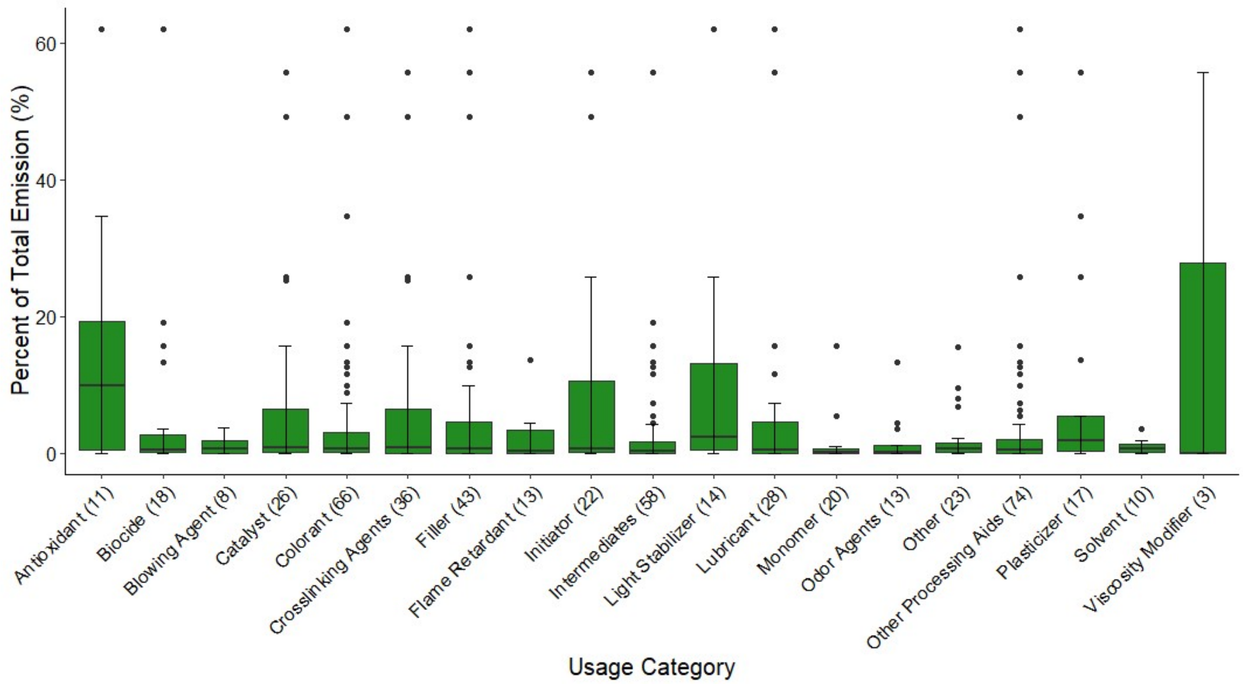

Figure S5: The partitioning into sludge of the 124 PMT plastic additives, based on their use category.

Table S4: Priority ranking of the 124 PMT plastic additives, ranked by total emission via effluent (with biodegradation). Substances with > 80% modeled emission through effluent are shaded orange, substances with > 50% < 80% modeled emission through effluent are shaded yellow.

Priority Rank	Name	CAS #	Total emission via effluent (%)
1	2-(1-methylpropyl)-4,6-dinitrophenol	88-85-7	99.9
2	2,2'-(1,2-ethenediyl)bis[5-amino-benzenesulfonic acid]	81-11-8	99.8
3	4-amino-benzenesulfonic acid	121-57-3	99.6
4	1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane	100-97-0	99.4
5	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(2,1-diazenediyl)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxo-butanamide]	5567-15-7	99.4
6	2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(2,1-diazenediyl)]bis[N-(2,4-dimethylphenyl)-3-oxo-butanamide]	22094-93-5	99.4
7	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(2,1-diazenediyl)]bis[N-(2-methylphenyl)-3-oxo-butanamide]	5468-75-7	99.3
8	2-methyl-4,6-bis[(octylthio)methyl]-phenol	110553-27-0	98.9
9	1,1'-(methylenedi-4,1-phenylene)bis-1H-Pyrrole-2,5-dione	13676-54-5	98.8
10	N-butyl-benzenesulfonamide	3622-84-2	98.8
11	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(2,1-	6358-37-8	98.1

	diazenediyl)]bis[N-(4-methylphenyl)-3-oxo-butanamide]		
12	2-amino-5-methyl-benzenesulfonic acid	88-44-8	97.1
13	N-[4-(2-oxiranylmethoxy)phenyl]-N-(2-oxiranylmethyl)-2-oxiranemethanamine	5026-74-4	97.1
14	6-chloro-N2-ethyl-N4-(1-methylethyl)-1,3,5-triazine-2,4-diamine	1912-24-9	97.0
15	1,1'-oxybis[2-methoxy-ethane]	111-96-6	96.4
16	2,4-dichlorophenol	120-83-2	96.2
17	1,1,1-trifluoro-methanesulfonic acid	1493-13-6	96.1
18	2-Chloro-, 1,1',1''-phosphate ethanol	115-96-8	95.8
19	1,8-Naphthalenediamine	479-27-6	95.6
20	2-methyl-1-[4-(methylthio)phenyl]-2-(4-morpholinyl)-1-propanone	71868-10-5	95.5
21	5,5-diphenyl-2,4-imidazolidinedione	57-41-0	95.4
22	1-chloro-4-nitrobenzene	100-00-5	95.1
23	1,4-Diazabicyclo[2.2.2]octane	280-57-9	95.0
24	1,1'-cyclohexylidenebis[2-(1,1-dimethylethyl)peroxide]	3006-86-8	94.4
25	1-methyl-4-nitro-benzene	99-99-0	93.9
26	2,4-diisocyanato-1-methyl-benzene	584-84-9	93.5
27	4,4'-sulfonylbis-benzenamine	80-08-0	93.3
28	1,3,5-Triazine-2,4,6(1H,3H,5H)-trione	108-80-5	93.3
29	4,4'-methylenebis[2-methyl-cyclohexanamine]	6864-37-5	93.3
30	4,4'-methylenebis(cyclohexylamine)	1761-71-3	93.2
31	4,4'-methylenebis-benzenamine	101-77-9	93.2
32	1-methyl-2-nitro-benzene	88-72-2	93.1
33	4,4'-oxybis-, 1,1'-dihydrazide benzenesulfonic acid	80-51-3	92.6
34	2,2'-(1,2-diazenediyl)bis[2-methyl-propanenitrile]	78-67-1	92.3
35	1,2-dibromoethane	106-93-4	91.9
36	4,4'-sulfonylbis-phenol	80-09-1	91.7
37	N,N'-bis(2-methylphenyl)-guanidine	97-39-2	91.6
38	N-methyl-benzenamine	100-61-8	91.4
39	Benzothiazole	95-16-9	91.1
40	4-ethenyl-pyridine	100-43-6	90.7
41	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	482-89-3	89.8
42	2,2,2-trifluoro-acetic acid	76-05-1	89.8
43	2-butoxy-, 1,1',1''-phosphate ethanol	78-51-3	89.5
44	Isoquinoline	119-65-3	89.4
45	(17α)-hydroxy-19-norpregn-4-en-20-yn-3-one	68-22-4	88.6
46	2,3,4,6,7,8,9,10-octahydro-pyrimido[1,2-a]azepine	6674-22-2	88.5
47	Dibutyl ester phosphoric acid	107-66-4	87.4
48	N-(4-hydroxyphenyl)-acetamide	103-90-2	87.4
49	2,4,6-tribromophenol	118-79-6	87.4

50	N,N-dimethyl-2-propenamide	284-95-7, 2680-03-7	87.2
51	1,1'-sulfinylbis-methane	CAS_RN:67-68-5	87.0
52	3-chloro-benzenamine	108-42-9	86.9
53	N1-[2-(dimethylamino)ethyl]-N1,N2,N2-trimethyl-1,2-ethanediamine	3030-47-5	86.6
54	1,4-dioxane	123-91-1	86.5
55	1,3-Dichloro-, 2,2',2''-phosphate 2-propanol	13674-87-8	86.1
56	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	81-07-2	84.9
57	2-nitropropane	79-46-9	84.4
58	(2-hydroxy-4-methoxyphenyl)phenyl-methanone	131-57-7	84.0
59	1,1,1,3,3,3-hexafluoro-2-Propanol	920-66-1	82.7
60	2-(2H-benzotriazol-2-yl)-4-methyl-phenol	2440-22-4	82.6
61	5,5'-(1H-isoindole-1,3(2H)-diylidene)bis-2,4,6(1H,3H,5H)-pyrimidinetrione	36888-99-0	82.2
62	2,6-dimethyl-benzenamine	87-62-7	81.8
63	2,4,7,9-tetramethyl-5-decyne-4,7-diol	126-86-3	80.9
64	Diphenyl-methanone	119-61-9	80.8
65	1-methyl-1-phenylethylhydroperoxide	80-15-9	78.9
66	2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonic acid	15214-89-8	77.6
67	4-aminophenol	CAS_RN:123-30-8	77.6
68	1,3,5-Triazine-2,4,6-triamine	CAS_RN:108-78-1	77.5
69	Nitrobenzene	CAS_RN:98-95-3	76.8
70	2,2'-oxybis[N,N-dimethyl-ethanamine]	CAS_RN:3033-62-3	74.7
71	N-cyanoguanidine	CAS_RN:461-58-5	73.3
72	N,N'-diphenyl-guanidine	102-06-7	72.7
73	5-amino-1,3,3-trimethyl-cyclohexanemethanamine	2855-13-2	72.3
74	N-ethyl-N-hydroxy-ethanamine	3710-84-7	69.9
75	5-chloro-2-(2,4-dichlorophenoxy)-phenol	3380-34-5	69.8
76	N,N'-diphenyl-thiourea	102-08-9	69.8
77	2,2'-(1,2-diazenediyl)bis[2-methyl-butanenitrile]	13472-08-7	69.3
78	N'-(3,4-dichlorophenyl)-N,N-dimethyl-urea	330-54-1	68.7
79	1-Chloro-, 2,2',2''-phosphate 2-propanol	13674-84-5	67.5
80	Triethyl ester phosphoric acid	78-40-0	66.6
81	Hexahydro-1,3-isobenzofurandione	85-42-7	66.5
82	N,N,N',N'-tetramethyl-thiodicarbonic diamide ([(H2N)C(S)]2S)	97-74-5	66.5
83	N,N-bis[2-[bis(carboxymethyl)amino]ethyl]-glycine	67-43-6	62.5
84	1,1'-oxybis-methane	115-10-6	60.8
85	Anthracene	120-12-7	57.4
86	1,2-dihydro-acenaphthylene	83-32-9	55.6
87	N,N'-1,2-ethanediylbis[N-(carboxymethyl)-glycine	60-00-4	52.5
88	1,1'-(phenylphosphinylidene)bis[1-(2,4,6-trimethylphenyl)-methanone	162881-26-7	50.1

89	1,2,3-trichloropropane	96-18-4	49.5
90	2-methyl-benzenesulfonamide	88-19-7	42.4
91	2-[[2-[2-(dimethylamino)ethoxy]ethyl]methylamino]-ethanol	83016-70-0	42.4
92	2-methoxy-2-methyl-propane	1634-04-4	41.5
93	Bis(1-methyl-1-phenylethyl) peroxide	80-43-3	40.2
94	Naphthalene	91-20-3	35.7
95	1H-Benzotriazole	95-14-7	35.5
96	1,1,2-trichloroethane	79-00-5	35.2
97	1,2-dichloroethane	107-06-2	28.5
98	1-bromo-3-chloropropane	109-70-6	24.8
99	1,2,4-trichlorobenzene	120-82-1	24.6
100	1,2,3-trichlorobenzene	87-61-6	21.5
101	1,2-dichlorobenzene	95-50-1	20.1
102	2,2'-oxybis-propane	108-20-3	17.2
103	1,2,3,4-tetrahydro-naphthalene	119-64-2	16.6
104	Chlorobenzene	108-90-7	14.8
105	3a,4,7,7a-tetrahydro-4,7-methano-1H-indene	77-73-6	14.6
106	1,3-dichlorobenzene	541-73-1	11.1
107	4-ethenyl-cyclohexene	100-40-3	9.4
108	Trichloromethane	67-66-3	8.7
109	1,3,5-trimethyl-benzene	108-67-8	7.8
110	(1-methylethyl)-benzene	98-82-8	6.9
111	1,1,2,2-tetrachloroethene	127-18-4	6.3
112	Tetrachloromethane	56-23-5	5.7
113	(1E)-1,2-dichloroethene	156-60-5	5.0
114	1,1,1,3,3,3-hexamethyl-disiloxane	107-46-0	4.3
115	1,1,1-trichloroethane	71-55-6	4.0
116	2,4,6,8-tetraethenyl-2,4,6,8-tetramethyl-cyclotetrasiloxane	2554-06-5	3.9
117	Dichlorodifluoromethane	75-71-8	3.4
118	1,2-dichloropropane	78-87-5	3.3
119	Chlorotrimethylsilane	75-77-4	0.6
120	Chloroethane	75-00-3	0.3
121	1,1-dichloroethylene	75-35-4	0.1
122	1,1,2-trichloroethene	79-01-6	0.0
123	Chloroethene	75-01-4	0.0
124	Chloromethane	74-87-3	0.0

Table S7: Comparison of modeled removal from a typical WWTP in this study to observed removal in the literature.

CAS	Name	Removal (%)	Removal (Literature, %)
95-14-7	1H-Benzotriazole	64.49	26[1-3], ~30[4], 56-74[5]
115-96-8	2-Chloro-, 1,1',1''-phosphate ethanol	4.23	1[1,6], ~20[4]
13674-84-5	1-Chloro-, 2,2',2''-phosphate 2-propanol	32.54	1[1,6], ~0[4]
13674-87-8	1,3-Dichloro-, 2,2',2''-phosphate 2-propanol	13.87	1[1,6]
78-51-3	2-butoxy-, 1,1',1''-phosphate ethanol	10.53	88[1,6]
3380-34-5	5-chloro-2-(2,4-dichlorophenoxy)-phenol	30.23	90[1,7-8], ~70[9]
95-16-9	Benzothiazole	8.89	80[1,3,10], ~80[4]
131-57-7	(2-hydroxy-4-methoxyphenyl)phenyl-methanone	15.97	90[1,11-12], ~70-100[9]
126-86-3	2,4,7,9-tetramethyl-5-decyne-4,7-diol	19.13	50[1,13]
103-90-2	N-(4-hydroxyphenyl)-acetamide	12.59	100[1,3,14-15], ~92-100[9], 73.4-99.3[16]
1981-07-02	1,2-benzisothiazol-3(2H)-one 1,1-dioxide	15.08	99[1,17-18]
60-00-4	N,N'-1,2-ethanediylbis[N-(carboxymethyl)-glycine	47.49	5[1,10,19-21], ~0[4]
1912-24-9	6-chloro-N2-ethyl-N4-(1-methylethyl)-1,3,5-triazine-2,4-diamine	2.97	23[1,3,22], ~0[5]
330-54-1	N'-(3,4-dichlorophenyl)-N,N-dimethyl-urea	31.34	33[1-3,22], ~0[5]
83-32-9	1,2-dihydro-acenaphthylene	44.4	85[1,23]
120-12-7	Anthracene	42.64	90[1,23]
91-20-3	Naphthalene	64.34	60[1,23]
108-78-1	1,3,5-Triazine-2,4,6-triamine	22.54	53[24]

References

1. J. Margot, L. Rossi, D. A. Barry and C. Holliger, A review of the fate of micropollutants in wastewater treatment plants, *Wiley Interdiscip. Rev. Water*, 2015, **2**, 457–487.
2. R. L. Oulton, T. Kohn and D. M. Cwiertny, Pharmaceuticals and personal care products in effluent matrices: A survey of transformation and removal during wastewater treatment and implications for wastewater management, *J. Environ. Monit.*, 2010, **12**, 1956–1978.
3. A. A. Guedez and W. Püttmann, Occurrence and fate of TMDD in wastewater treatment plants in Germany, *Water Res.*, 2011, **45**, 5313–5322.
4. T. Reemtsma, S. Weiss, J. Mueller, M. Petrovic, S. González, D. Barcelo, F. Ventura and T. P. Knepper, Polar pollutants entry into the water cycle by municipal wastewater: A European perspective, *Environ. Sci. Technol.*, 2006, **40**, 5451–5458.
5. W. Qi, H. Singer, M. Berg, B. Müller, B. Pernet-Coudrier, H. Liu and J. Qu, Elimination of polar micropollutants and anthropogenic markers by wastewater treatment in Beijing, China, *Chemosphere*, 2015, **119**, 1054–1061.

6. K. D. North, Tracking Polybrominated Diphenyl Ether Releases in a Wastewater Treatment Plant Effluent, Palo Alto, California, *Environ. Sci. Technol.*, 2004, **38**, 4484–4488.
7. M. Gardner, S. Comber, M. D. Scrimshaw, E. Cartmell, J. Lester and B. Ellor, The significance of hazardous chemicals in wastewater treatment works effluents, *Sci. Total Environ.*, 2012, **437**, 363–372.
8. M. Pelaez, M. G. Antoniou, X. He, D. D. Dionysiou, A. A. De Cruz, K. Tsimeli, T. Triantis, T. Kaloudis, C. Williams, M. Aubel, A. Foss, U. Khan, K. E. O. Shea and J. Westrick, 2010, vol. 16, pp. 213–226.
9. B. Kasprzyk-Hordern, R. M. Dinsdale and A. J. Guwy, The removal of pharmaceuticals, personal care products, endocrine disruptors and illicit drugs during wastewater treatment and its impact on the quality of receiving waters, *Water Res.*, 2009, **43**, 363–380.
10. M. G. Kokotou and N. S. Thomaidis, Determination of eight artificial sweeteners in wastewater by hydrophilic interaction liquid chromatography-tandem mass spectrometry, *Anal. Methods*, 2013, **5**, 3825–3833.
11. L. Bijlsma, E. Emke, F. Hernández and P. De Voogt, Investigation of drugs of abuse and relevant metabolites in Dutch sewage water by liquid chromatography coupled to high resolution mass spectrometry, *Chemosphere*, 2012, **89**, 1399–1406.
12. J. J. Yang and C. D. Metcalfe, Fate of synthetic musks in a domestic wastewater treatment plant and in an agricultural field amended with biosolids, *Sci. Total Environ.*, 2006, **363**, 149–165.
13. J. E. Loyo-Rosales, C. P. Rice and A. Torrents, Fate of octyl- and nonylphenol ethoxylates and some carboxylated derivatives in three American wastewater treatment plants, *Environ. Sci. Technol.*, 2007, **41**, 6815–6821.
14. M. Clara, G. Windhofer, P. Weilgony, O. Gans, M. Denner, A. Chovanec and M. Zessner, Identification of relevant micropollutants in Austrian municipal wastewater and their behaviour during wastewater treatment, *Chemosphere*, 2012, **87**, 1265–1272.
15. R. Loos, R. Carvalho, D. C. António, S. Comero, G. Locoro, S. Tavazzi, B. Paracchini, M. Ghiani, T. Lettieri, L. Blaha, B. Jarosova, S. Voorspoels, K. Servaes, P. Haglund, J. Fick, R. H. Lindberg, D. Schwesig and B. M. Gawlik, EU-wide monitoring survey on emerging polar organic contaminants in wastewater treatment plant effluents, *Water Res.*, 2013, **47**, 6475–6487.
16. M. Papageorgiou, C. Kosma and D. Lambropoulou, Seasonal occurrence, removal, mass loading and environmental risk assessment of 55 pharmaceuticals and personal care products in a municipal wastewater treatment plant in Central Greece, *Sci. Total Environ.*, 2016, **543**, 547–569.
17. I. González-Mariño, J. B. Quintana, I. Rodríguez and R. Cela, Evaluation of the occurrence and biodegradation of parabens and halogenated by-products in wastewater by accurate-mass liquid chromatography-quadrupole-time-of-flight-mass spectrometry (LC-QTOF-MS), *Water Res.*, 2011, **45**, 6770–6780.
18. N. Lozano, C. P. Rice, M. Ramirez and A. Torrents, Fate of Triclocarban, Triclosan and Methyltriclosan during wastewater and biosolids treatment processes, *Water Res.*, 2013, **47**, 4519–4527.
19. G. G. Ying, B. Williams and R. Kookana, Environmental fate of alkylphenols and alkylphenol ethoxylates—a review, *Environ. Int.*, 2002, **28**, 215–226.

20. F. T. Lange, M. Scheurer and H. J. Brauch, Artificial sweeteners--a recently recognized class of emerging environmental contaminants: a review, *Anal. Bioanal. Chem.*, 2012, **403**, 2503–2518.
21. A. Bergé, M. Cladière, J. Gasperi, A. Coursimault, B. Tassin and R. Moilleron, Meta-analysis of environmental contamination by phthalates, *Environ. Sci. Pollut. Res. Int.*, 2013, **20**, 8057–8076.
22. J. Meyer and K. Bester, Organophosphate flame retardants and plasticisers in wastewater treatment plants, *J. Environ. Monit.*, 2004, **6**, 599–605.
23. M. Blanchard, M. J. Teil, D. Ollivon, L. Legenti and M. Chevreuil, Polycyclic aromatic hydrocarbons and polychlorobiphenyls in wastewaters and sewage sludges from the Paris area (France), *Environ. Res.*, 2004, **95**, 184–197.
24. H. Zhu and K. Kannan, Occurrence and distribution of melamine and its derivatives in surface water, drinking water, precipitation, wastewater, and swimming pool water, *Environ. Pollut.*, 2020, **258**, 113743.