Polyamide microplastics in wastewater as vectors of cationic pharmaceutical drugs. [Dataset]

WAGSTAFF, A., LAWTON, L.A. and PETRIE, B.

2022

Electronic supplementary material

Polyamide microplastics in wastewater as vectors of cationic pharmaceutical drugs

Antony Wagstaff, Linda A Lawton, Bruce Petrie*

School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen, AB10 7GJ, UK

*Email: b.r.petrie@rgu.ac.uk

The electronic supplementary information contains four figures and two tables which includes pharmaceutical recoveries through different filters, isotherm data, pharmaceutical log D_{OW} values and drug speciation at varying pH, the MS/MS instrumental parameters, and the *p*-values from the statistical analysis.

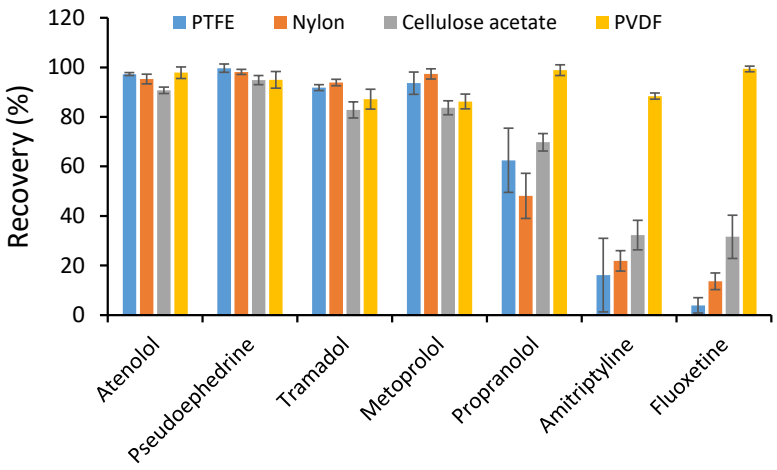

Figure S1. Recovery of pharmaceuticals through different membrane filters

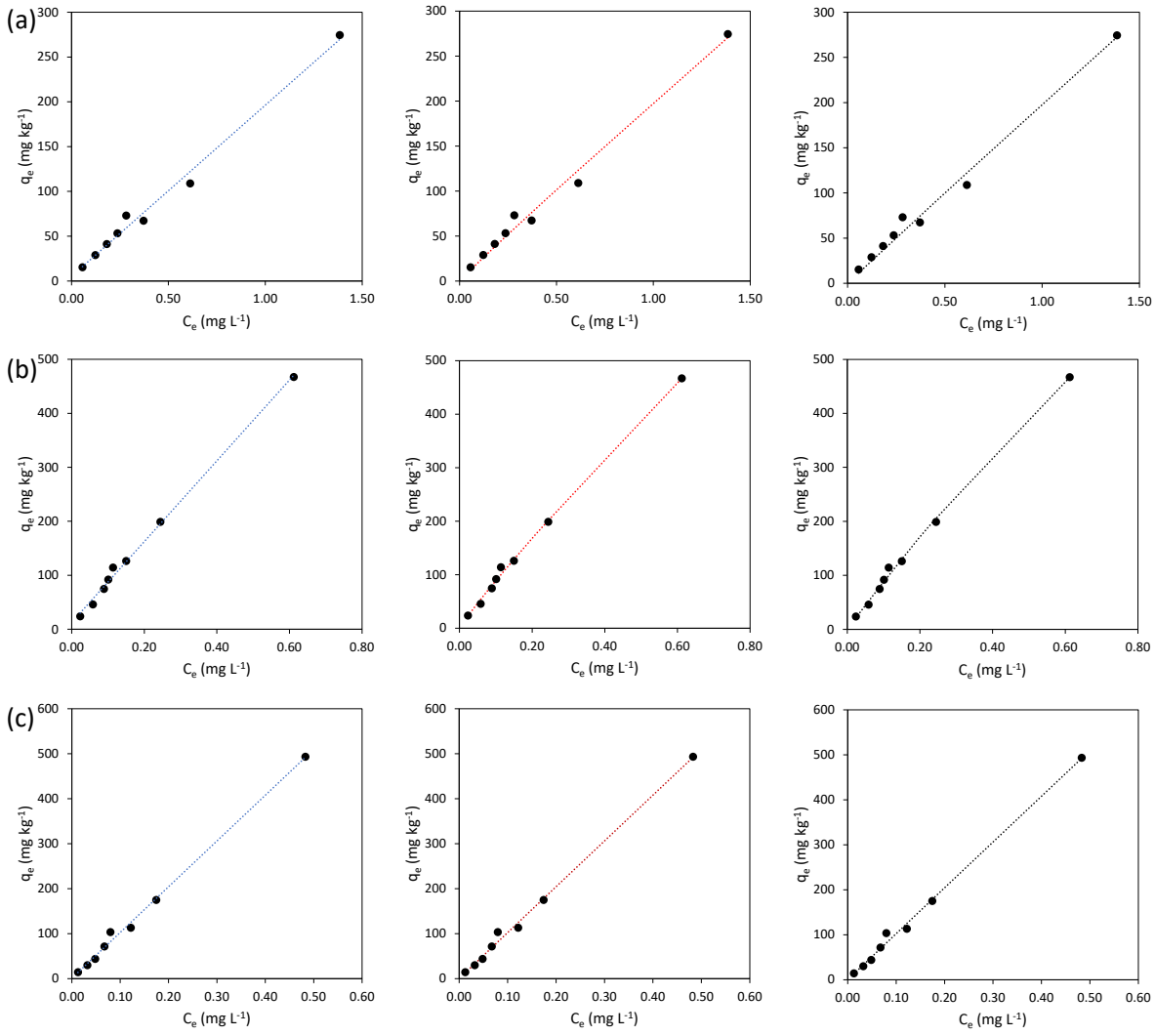

Figure S2. Equilibrium data of propranolol (a), amitriptyline (b), and fluoxetine (c) fitted to linear (blue dashed line), Freundlich (red dashed line) and Langmuir (black dashed line) isotherm models. The data points show the experimental data.

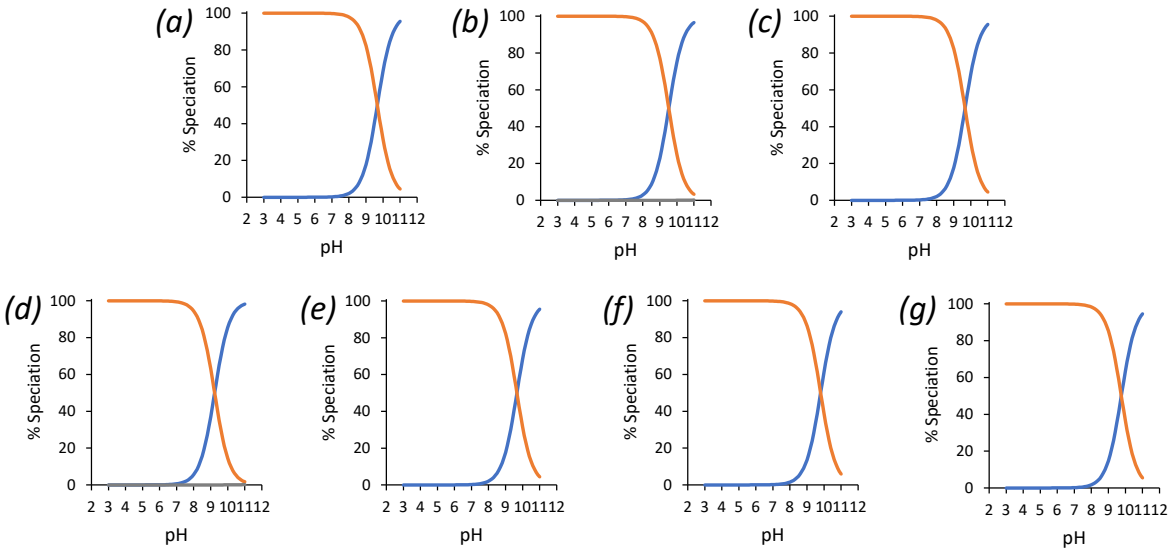

Figure S3. Speciation of atenolol *(A)*, pseudoephedrine *(B)*, metoprolol *(C)*, tramadol *(D)*, propranolol *(E)*, fluoxetine *(F)*, and amitriptyline *(G)* at different pH values. The orange line represents the positively charged species and the blue line represents the uncharged (neutral) species

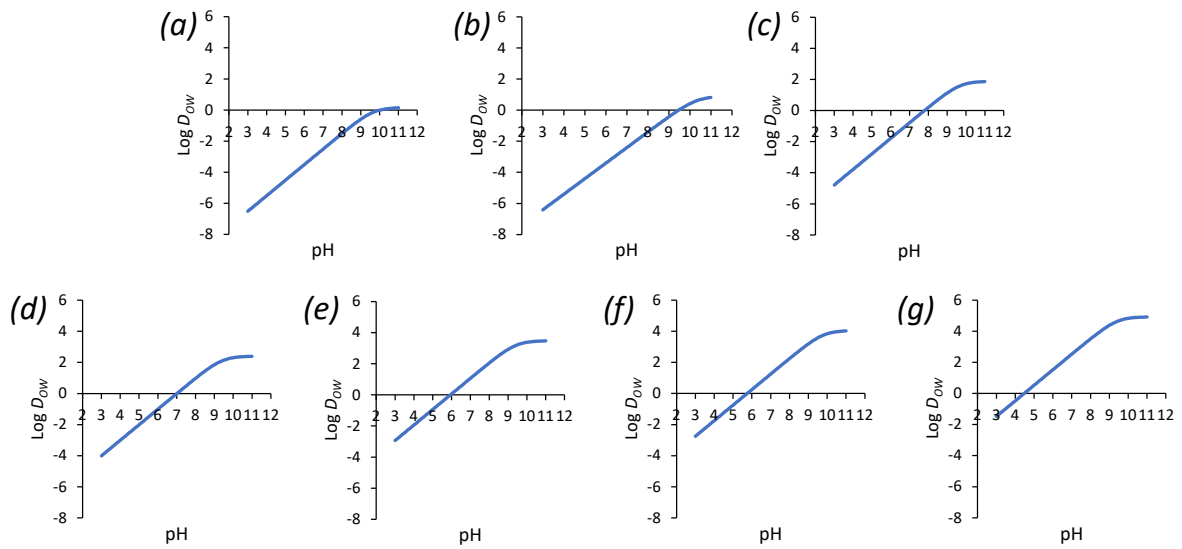

Figure S4. Log D_{OW} of atenolol *(A)*, pseudoephedrine *(B)*, metoprolol *(C)*, tramadol *(D)*, propranolol *(E)*, fluoxetine *(F)*, and amitriptyline *(G)* at different pH values

Table S1. MS/MS parameters of all pharmaceuticals, including those used as internal standards

Pharmaceutical	***R*$_t$ (minutes)**	**Precursor (m/z)**	**Fragmentor (V)**	**Product 1 (m/z)**	**CE (eV)**	**Product 2 (m/z)**	**CE (eV)**	**Internal standard**
Atenolol	3.4	266.9	110	189.9	20	145.0	30	Codeine
Pseudoephedrine	4.2	166.0	90	148.0	10	91.0	40	Codeine
Metoprolol	8.7	268.1	110	191.1	10	116.0	12	Acebutolol
Tramadol	8.5	264.1	90	58.1	20	-	-	Acebutolol
Propranolol	10.6	259.9	110	182.9	10	115.9	10	Carbamazepine
Fluoxetine	12.4	309.8	90	147.7	2	44.0	10	Carbamazepine
Amitriptyline	12.1	278.1	100	233.1	10	91.0	30	Carbamazepine
Codeine[a]	4.8	300.0	100	214.9	20	-	-	-
Acebutolol[a]	8.8	337.2	90	116.1	20	-	-	-
Carbamazepine[a]	11.5	236.8	130	193.9	20	-	-	-

Key: R_t, retention time; CE, collision energy

[a]Internal standard

Table S2. Adjusted *p*-values from the statistical analysis

Wastewater parameters compared	Propranolol	Amitriptyline	Fluoxetine
	Adjusted *p*-value	**Adjusted *p*-value**	**Adjusted *p*-value**
One-way ANOVA followed by Tukey's post-hoc multiple comparisons test			
pH 3 *vs*. pH 6	0.8663	0.0145	0.0002
pH 3 *vs*. pH 7	0.1247	<0.0001	<0.0001
pH 3 *vs*. pH 8	0.0478	<0.0001	<0.0001
pH 3 *vs*. pH 11	<0.0001	<0.0001	<0.0001
pH 6 *vs*. pH 7	0.4572	0.0008	0.0002
pH 6 *vs*. pH 8	0.2039	<0.0001	<0.0001
pH 6 *vs*. pH 11	<0.0001	<0.0001	<0.0001
pH 7 *vs*. pH 8	0.9676	0.3084	0.0534
pH 7 *vs*. pH 11	0.0004	<0.0001	<0.0001
pH 8 *vs*. pH 11	0.0008	<0.0001	<0.0001
100% wastewater *vs*. 75% wastewater	>0.9999	0.0878	0.0005
100% wastewater *vs*. 50% wastewater	0.3937	0.0052	0.0014
100% wastewater *vs*. 25% wastewater	0.0044	0.0019	0.0006
100% wastewater *vs*. 0% wastewater	0.0009	0.0019	0.0032
75% wastewater *vs*. 50% wastewater	0.4436	0.3943	0.9216
75% wastewater *vs*. 25% wastewater	0.0051	0.1472	0.9993
75% wastewater *vs*. 0% wastewater	0.001	0.1522	0.6315
50% wastewater *vs*. 25% wastewater	0.0742	0.9463	0.9743
50% wastewater *vs*. 0% wastewater	0.0125	0.9518	0.9708
25% wastewater *vs*. 0% wastewater	0.776	>0.9999	0.7561
0 g/L NaCl *vs*. 1 g/L NaCl	0.0028	0.7227	0.5886
0 g/L NaCl *vs*. 2 g/L NaCl	0.0059	0.9999	0.3604
0 g/L NaCl *vs*. 3 g/L NaCl	0.0034	0.9979	0.6205
0 g/L NaCl *vs*. 4 g/L NaCl	0.004	0.8632	0.2244
1 g/L NaCl *vs*. 2 g/L NaCl	0.9831	0.7961	0.9909
1 g/L NaCl *vs*. 3 g/L NaCl	>0.9999	0.5537	0.0874
1 g/L NaCl *vs*. 4 g/L NaCl	0.9988	0.9983	0.9254
2 g/L NaCl *vs*. 3 g/L NaCl	0.9942	0.9909	0.0442
2 g/L NaCl *vs*. 4 g/L NaCl	0.9988	0.9157	0.9959
3 g/L NaCl *vs*. 4 g/L NaCl	>0.9999	0.7139	0.0254
Unpaired t-test followed by Welch's correction			
20 °C *vs*. 5 °C	0.0095	0.001	0.0035