Optimisation of the analysis of anti-influenza drugs in wastewater and surface water

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Table S1. Chemical structures and physicochemical properties of anti-influenza drugs examined in this study [1-11].

Compound	Molecular formula	Molecular mass (g/mol)	Structure	pK _a	LogP	Excretion (%)
Oseltamivir (OS)	C ₁₆ H ₂₈ N ₂ O ₄	312.41		7.7 [1.2]	0.36 [1]	15 [9]
Oseltamivir carboxylate (OC)	C ₁₄ H ₂₄ N ₂ O ₄	284.35		3.78 (acid) [3.4] 7.76 (base) [3.4]	-2.1 [6]	80 [9]
Zanamivir (ZAN)	C ₁₂ H ₂₀ N ₄ O ₇	332.31		3.82 (acid) [4] 11.26 (base) [4]	-7.13 [7]	80 [10]
Amantadine (AMN)	C ₁₀ H ₁₇ N	151.24		10.1 [5]	2.44 [8]	78 [11]

Table S2. Evaluation of solid-phase extraction cartridges and elution solvents.

Cartridge	Elution solvent	Recovery rate (%)			
		OS	OC	ZAN	AMN
Oasis HLB (200 mg)	A	45.0	49.2	4.0	54.5
	B	51.8	102.2	6.8	54.8
Oasis MCX (150 mg)	A	56.9	79.0	4.5	22.0
	B	53.3	87.3	38.0	0
ISOLUTE ENV+ (500 mg)	B	20.8	49.3	13.1	0
Bond Elut SCX (100 mg)	B	68.7	77.0	51.8	67.9
	C	45.2	49.3	36.7	54.1
	D	43.9	43.1	7.3	15.4
	E	39.4	55.9	11.4	48.8
Bond Elut Plexa PCX (200 mg)	B	40.3	88.7	5.1	33.3
Bond Elut PRS (200 mg)	B	39.1	76.2	12.4	42.4
	C	39.4	66.8	9.4	66.6
	D	34.5	47.2	4.0	13.0
	E	23.3	51.2	7.1	41.2
Bond Elut SAX (200 mg)	F	30.2	19.4	0	12.6
Discovery DSC SCX (500 mg)	B	29.4	46.5	14.6	58.1
Supelclean LC SCX (500 mg)	B	13.1	29.4	1.5	20.7
Strata SCX (500 mg)	B	36.9	47.2	41.4	24.2
Strata X-C (500 mg)	B	30.5	93.0	4.4	0.3
ISOLUTE SCX (500 mg)	B	18.9	41.5	11.1	25.0
InertSep LSC SCX2 (500 mg)	B	24.9	59.4	0	31.6
HyperSep SCX (500 mg)	B	54.3	91.7	22.8	67.3
HyperSep Retain CX (500 mg)	B	17.0	79.6	17.0	1.8

Elution solvents : (A) methanol containing 2% ammonia (v/v); (B) 10% triethylamine in a 1:1 (v/v) mixture of acetone and water; (C) 10% triethylamine in a 1:1 (v/v) mixture of methanol and water; (D) 10% ammonia in a 1:1 (v/v) mixture of acetone and water; (E) 10% ammonia in a 1:1 (v/v) mixture of methanol and water; and (F) methanol containing 2% acetic acid.

Figure S1. Effects of application flow speed (mL min⁻¹) on recovery rates of target compounds in 50 mL of MilliQ-based water.

Figure S2. Effects of sample volume on recovery rates of analytes in STP influent. Each sample volume specified in the figure was applied to a Bond Elut SCX cartridge containing 500 mg of adsorbent.

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