

Original Article

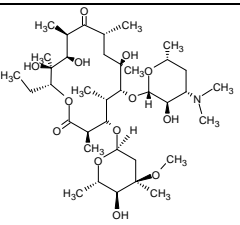
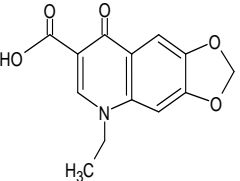
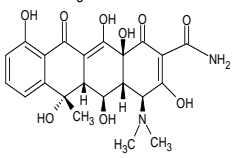
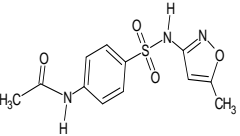
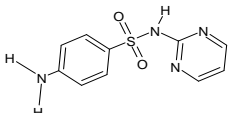
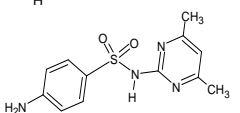
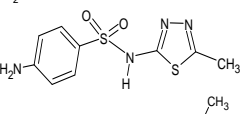
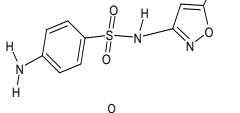
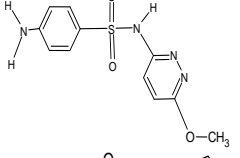
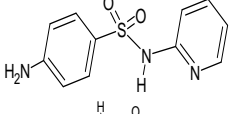
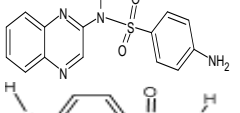
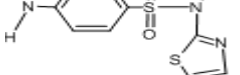
Detection of pharmaceuticals and their transformation products in seawaters using off-line solid phase extraction and liquid chromatography-high resolution mass spectrometry

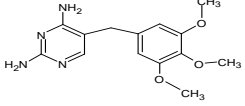
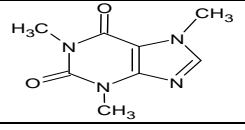
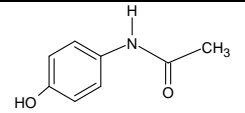
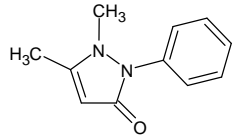
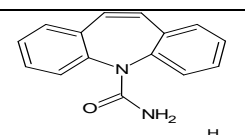
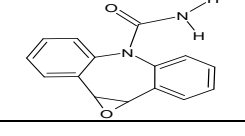
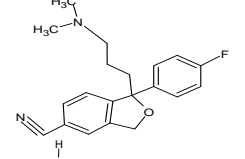
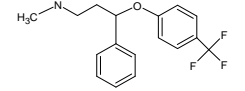
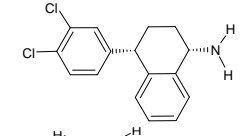
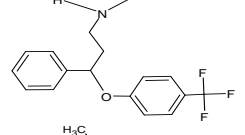
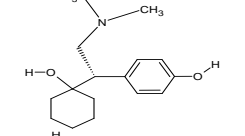
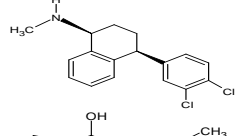
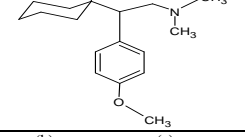
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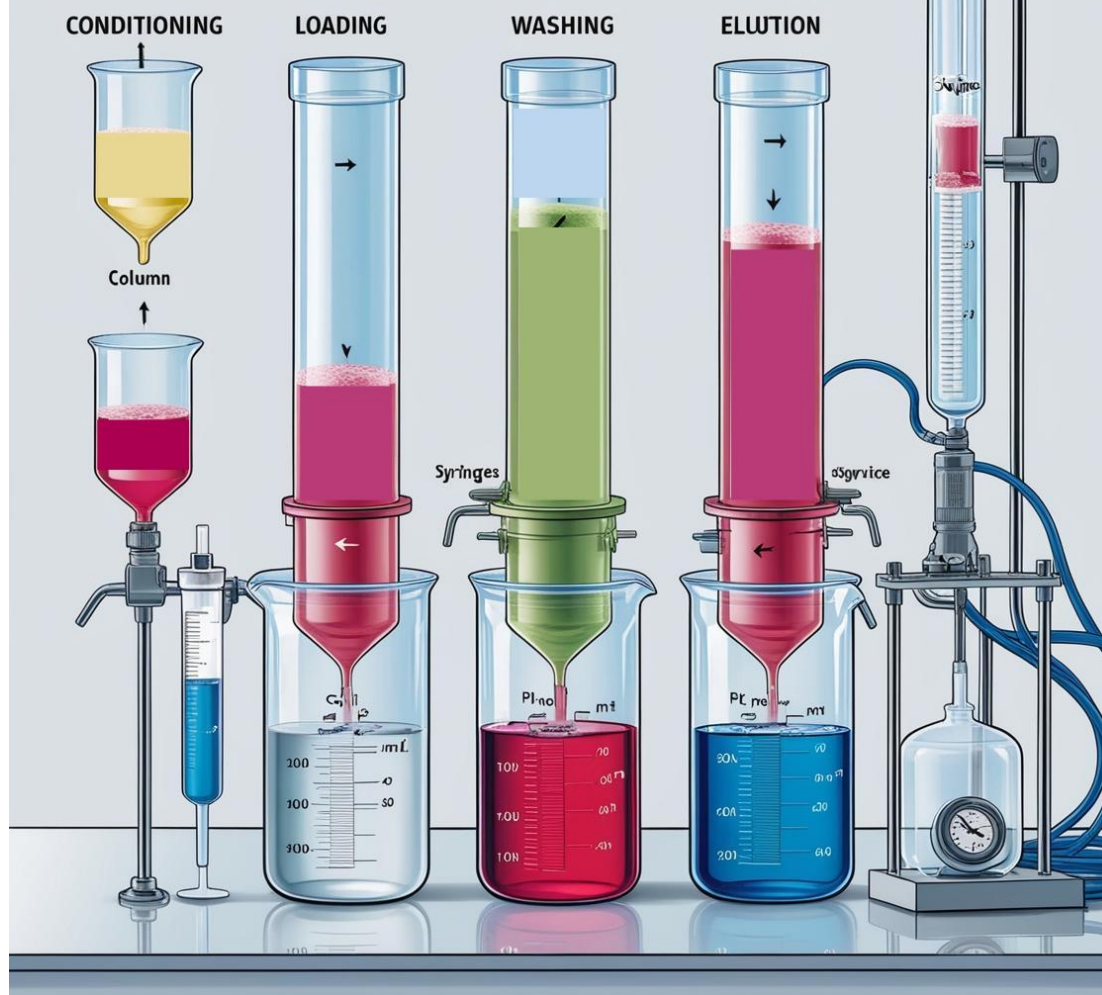
Table S1. Molecular structure and chemical properties of the selected pharmaceuticals

Compound	Molecular structure ^a	MW ^a (g/mol)	Water Solubility ^a (mg/l)	pKa ^a (25°C)	logKow ^a
Antibiotics					
Erythromycin- H ₂ O		733.937	2000	8.88	3.06
Oxolinic acid		261.233	0.003	5.58 ^b	0.94
Oxytetracycline		460.439	313 (25°C)	3.27	-0.9
N acetyl sulfamethoxazole (TP)		295.313	631	5.88	0.86
Sulfadiazine		250.276	<1000	6.36	-0.09
Sulfamethazine		278.33	230	7.59	0.14
Sulfamethizole		270.325	611	2.1	0.54
Sulfamethoxazole		253.276	610 (37°C)	1.6/5.7 ^c	0.89
Sulfamethoxypyridazin e		280.302	325	6.7	0.32
Sulfapyridine		249.288	235	8.43	0.35
Sulfaquinoxaline		300.336	76.1	5.1	1.68
Sulfathiazole		255.31	921	7.2	0.05

Trimethoprim		290.323	400 (25°C)	7.12(20°C)/ 7.2 ^{b,c}	0.91/1.33 ^b
Stimulant					
Caffeine		194.194	16000 (25°C)	14/10.4 ^d	-0.07
Analgesics					
Paracetamol		151.165	14000 (20°C)	9.38 ^d	0.46
Phenazone		188.23	47400	1.5	0.46
Anticonvulsant					
Carbamazepine		236.274	152	7/13.9 ^c	1.51
Carbamazepine-10,11-epoxide		252.273	1340	3.7/19.65 ^d	1.97
Antidepressants					
Citalopram		324.399	5.88	9.78 ^e	3.74
Fluoxetine		309.332	1.7x10 ⁻³	9.8	1.22
N-desmethyl sertraline (TP)		292.203	0.0979	9.13	4.88
Norfluoxetine (TP)		295.305	9.15	9.77	3.74
O desmethyl venlafaxine (TP)		263.381	3700 (20°C)	9.45	2.72
Sertraline		306.230	3.5	9.85	1.37
Venlafaxine		277.408	230	8.91/14.42 ^e	10.09

Literature data from: ^(a)pubchem, ^(b)drugbank, ^(c)Verlicchi et al. [75], ^(d)Kosma et al. [4], ^(e)Huerta et al. [26]
(TPs): transformation product

SOLID PHASE EXTRACTION



↓
5 ml MeOH
5 ml H₂O

↓
250 sample
5 ml EDTA 5%
pH: 3

↓
5 ml H₂O

↓
2 × 5 ml MeOH

Figure S1. Optimized method for solid phase extraction (SPE) analysis