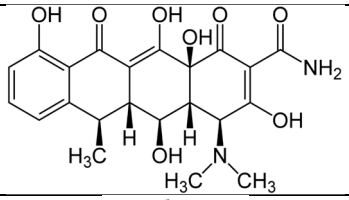
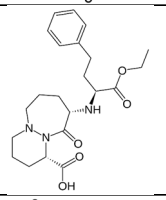
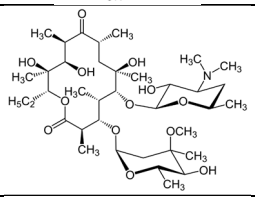
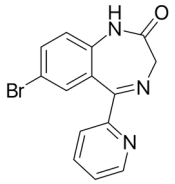
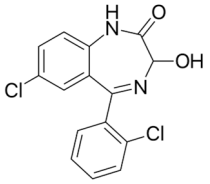
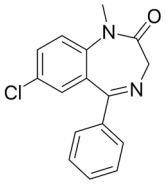
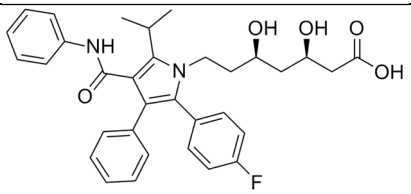
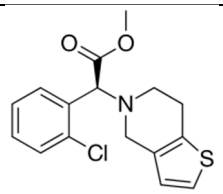
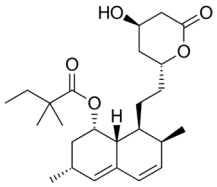
Modified fly ash as an adsorbent for the removal of pharmaceutical residues from water

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Table S1. Chemical structure of pharmaceuticals

Pharmaceutical	Chemical structure	WS, mg/dm^3	pKa	$logK_{ow}$
Doxycycline		630	3.5, 7.7, 9.5	-0.02
Cilazapril		27.5	3.41 5.35	2.27
Erythromycin		1.4	8.88	3.06
Bromazepam		175	2.65 12.24	2.05
Lorazepam		80.8	13	2.39
Diazepam		50.0	3.40	2.82
Atorvastatin		$1.1 \cdot 10^{-3}$	4.46	6.36

Clopidogrel		50.8	4.77	3.82
Simvastatin		0.03	-2.8 14.9	4.68

HPLC-MS/MS analysis of pharmaceuticals

The pharmaceutical concentration was monitored by HPLC-MS/MS. The pharmaceuticals were separated using an HPLC system on a Zorbax Eclipse XDB-C18 reversed-phase column, which was 75 mm long and 4.6 mm in internal diameter and had a 3.5 μm particle size (Agilent Technologies). The mobile phase used in these experiments consisted of water (A), methanol (B), and 10% acetic acid (C), and the gradient of the mobile phase is presented in Table S2.

Table S2. Gradient and flow rate of the mobile phase

Time, min	Flow rate, cm^3min^{-1}	A, %	B, %	C, %
0	0.5	38	60	2
8.00	0.5	0	98	2
15.00	0.5	0	98	2
15.01	0.9	0	100	0
18.00	0.9	0	100	0
18.01	0.5	38	60	2
20.00	0.5	38	60	2

An LTQ XL mass spectrometer with a linear ion trap was used for the detection and quantification of the pharmaceutical preparations. The electrospray ionization technique was used, and all the pharmaceuticals were analyzed in the positive ionization mode. Based on the obtained MS^2 spectra, the most intense fragment ions were selected, while the SRM mode was selected for the quantification of the tested pharmaceuticals. Table S3 shows the parameters of the instrumental method for the quantitative determination of the pharmaceuticals.

Table S3. HPLC-MS/MS parameters for quantitative determination of pharmaceuticals

Pharmaceutical	**Retention time, min**	**$[M+H]^+$**	**Colision energy, %**	**Product ion insulation range**
Doxycycline	2.76	445.00	25	427.0-429.0
Cilazapril	2.94	418.00	23	210.0-212.0
Erythromycin	2.95	734.10	26	575.0-577.0
Bromazepam	3.62	316.10	36	287.6-288.6
Lorazepam	4.51	321.00	32	302.4-303.4

Diazepam	6.22	285.20	40	256.7-257.7
Atorvastatin	6.91	559.00	25	465.0-467.0
Clopidogrel	8.15	321.90	28	210.8-212.8
Simvastatin	10.17	418.90	21	283.9-285.9

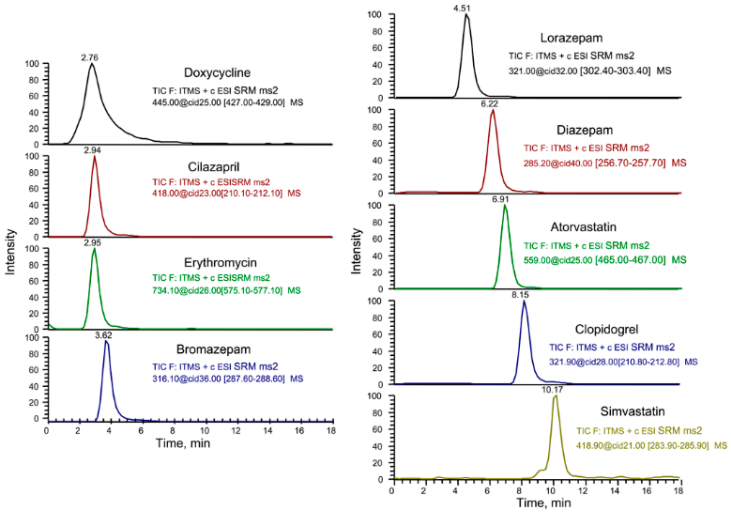


Figure S1. Mass chromatogram of selected pharmaceuticals.