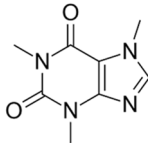
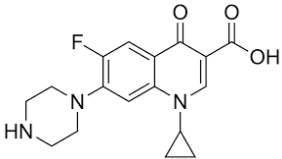
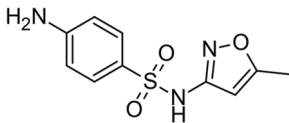
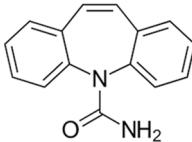


*Supplementary Information*

**Pharmaceutical Residues in Sediments of a Coastal Lagoon in Northwest Mexico—Occurrence and Environmental Risk Assessment**

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**Table S1.** Physical and chemical properties of the target PhACs

Compound	Structure	pK <sub>a</sub>	log K <sub>ow</sub>	Water solubility (g L <sup>-1</sup> )	log D at pH = 8.4 <sup>a</sup>	Henry's Law constant (atm m <sup>3</sup> mol <sup>-1</sup> )
Caffeine		14	-1.32	21.7	-1.32	$1.1 \times 10^{-11}$
Ciprofloxacin		pK <sub>a1</sub> = 6.09 pK <sub>a2</sub> = 8.62	0.28	25	0.044	$5.09 \times 10^{-19}$
Sulfamethoxazole		pK <sub>a1</sub> = 1.85 pK <sub>a2</sub> = 5.6	0.89	0.61	1.92	$6.4 \times 10^{-13}$
Carbamazepine		14	2.77	0.018	3.03	$1.08 \times 10^{-7}$

<sup>a</sup> For calculations of the logD values, a pH = 8.4 was used as it is the average pH value of marine water in the site where sediment samples were collected

**Table S2.** Validation parameters of the analytical method to quantify the analytes in sediment samples

Parameter	n	Caffeine	Ciprofloxacin	Sulfamethoxazole	Carbamazepine
Recovery (%)					
30 ng g <sup>-1</sup>	3	87.7-95.1	98-103	102-106	94.6-100
75 ng g <sup>-1</sup>	3	86.2-91.4	95-101	97.5-104	96.9-102
125 ng g <sup>-1</sup>	3	79.3-90.8	92-99.3	99.3-102	95.9-104
Precision (% , RSD)					
50 ng g <sup>-1</sup>	5	3.5-4.4	3.7-4.9	3.6-4.4	2.5-2.8
100 ng g <sup>-1</sup>	5	1.9-3.2	2.4-3.2	2.0-2.7	1.8-2.9
LOD (ng g <sup>-1</sup> )	-	0.25	0.5	0.5	0.25
LOQ (ng g <sup>-1</sup> )	-	1	2	2	1

**Table S3.** Determination of predicted no-effect concentration (PNEC) of the target PhACs for aquatic species from different trophic levels using different endpoints in chronic toxicity assays (Beiras, 2021).

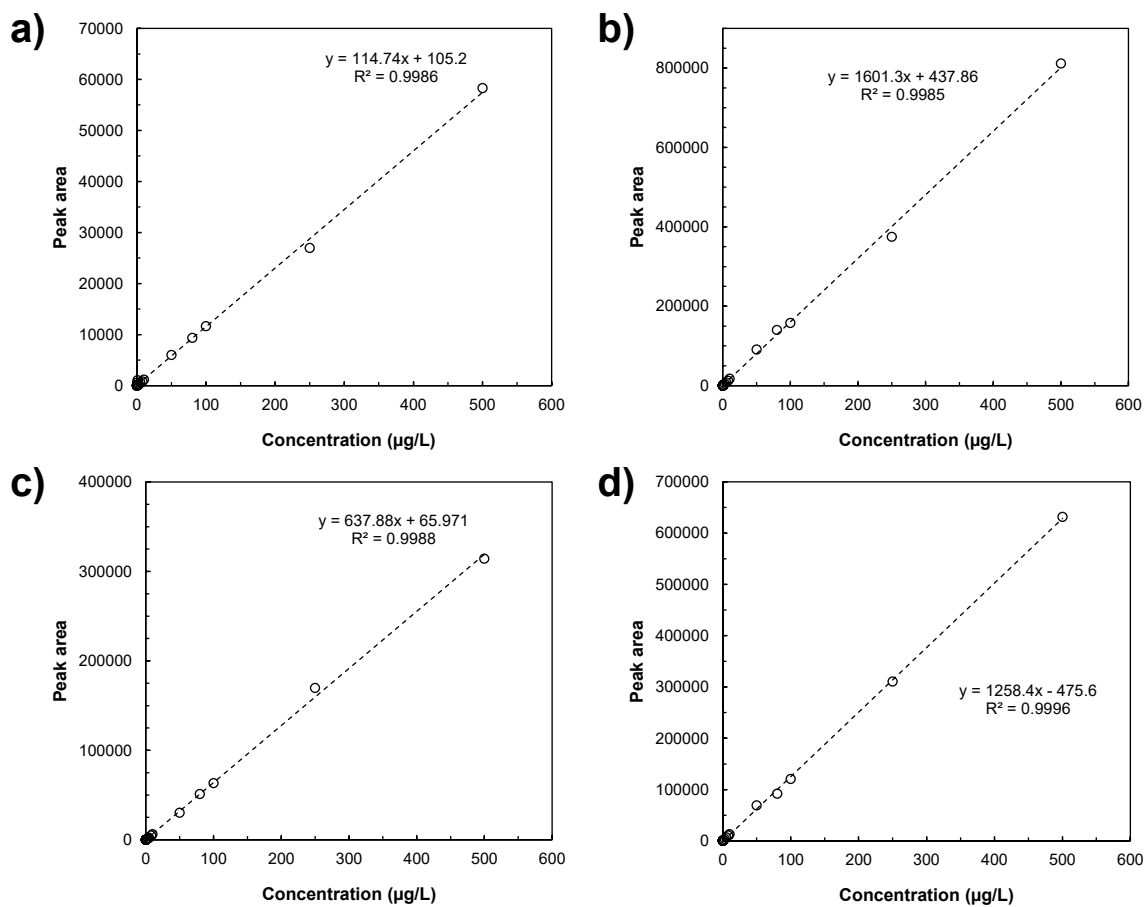
Compound	Species	Endpoint	Toxicity threshold	AF	PNEC (ng L <sup>-1</sup> )
Caffeine	<i>I. galbana</i>	Population growth (3 d)	EC <sub>10</sub>	100	192000
	<b><i>D. magna</i></b>	<b>Reproduction (21 d)</b>	<b>NOEC</b>	<b>100</b>	<b>1200</b>
	<i>P. promelas</i>	Mortality (7 d)	EC <sub>50</sub>	100	183330
Carbamazepine	<i>R. subcapitata</i>	Population growth (3 d)	EC <sub>10</sub>	100	6000
	<i>C. dubia</i>	Reproduction (7 d)	LOEC	100	1000
	<b><i>D. rerio</i></b>	<b>Reproduction 42 d)</b>	<b>LOEC</b>	<b>100</b>	<b>5</b>
Ciprofloxacin	<b><i>M. aeruginosa</i></b>	<b>Population growth (7 d)</b>	<b>EC<sub>50</sub></b>	<b>100</b>	<b>17</b>
	<i>D. magna</i>	Neonate immobilization (2 d)	NOEC	100	600000
	<i>P. promelas</i>	Survival and growth (7 d)	EC <sub>50</sub>	100	33330
Sulfamethoxazole	<b><i>C. neogracile</i></b>	<b>Cell density (20 d)</b>	<b>LOEC</b>	<b>100</b>	<b>0.75</b>
	<i>C. dubia</i>	Reproduction (7 d)	EC <sub>50</sub>	100	700
	<i>O. latipes</i>	Mortality (4 d)	LC <sub>50</sub>	1000	>333330

The PNEC values in bold were used to determine the risk quotients under the approach of the worst-case scenario

**Table S4.** Predicted no effect concentrations of the target PhACs for different trophic levels in the aquatic environment and their adaptation for sediments

<b>Compound</b>	<b>PNEC<sub>water</sub> (ng L<sup>-1</sup>)</b>	<b>K<sub>d</sub> (L kg<sup>-1</sup>)</b>	<b>PNEC<sub>sediment</sub> (ng g<sup>-1</sup>)</b>
Caffeine	1200	4.9 <sup>a</sup>	4,667
Carbamazepine	5	12.6 <sup>b</sup>	50
Sulfamethoxazole	0.75	8.9 <sup>c</sup>	5.29
Ciprofloxacin	17	37.05 <sup>d</sup>	500

<sup>a</sup>(da Costa Filho et al., 2022), <sup>b</sup>(Azuma et al., 2017), <sup>c</sup>(Xu et al., 2009), <sup>d</sup>(Gibs et al., 2013)



**Figure S1.** Matrix-matched calibration curves of the analytes: a) carbamazepine, b) sulfamethoxazole, c) ciprofloxacin, and d) caffeine

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