

Evaluation of Environmental Risks Posed by Pharmaceutically Active Compounds in the Great Bačka Canal

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✓ Aquatic ecosystems, including surface water bodies such as rivers, lakes, and canals are increasingly threatened by a wide array of pollutants, among which contaminants of emerging concern (CECs) have garnered significant attention due to their persistence, bioaccumulative potential, and sub-lethal effects on aquatic biota and water quality.

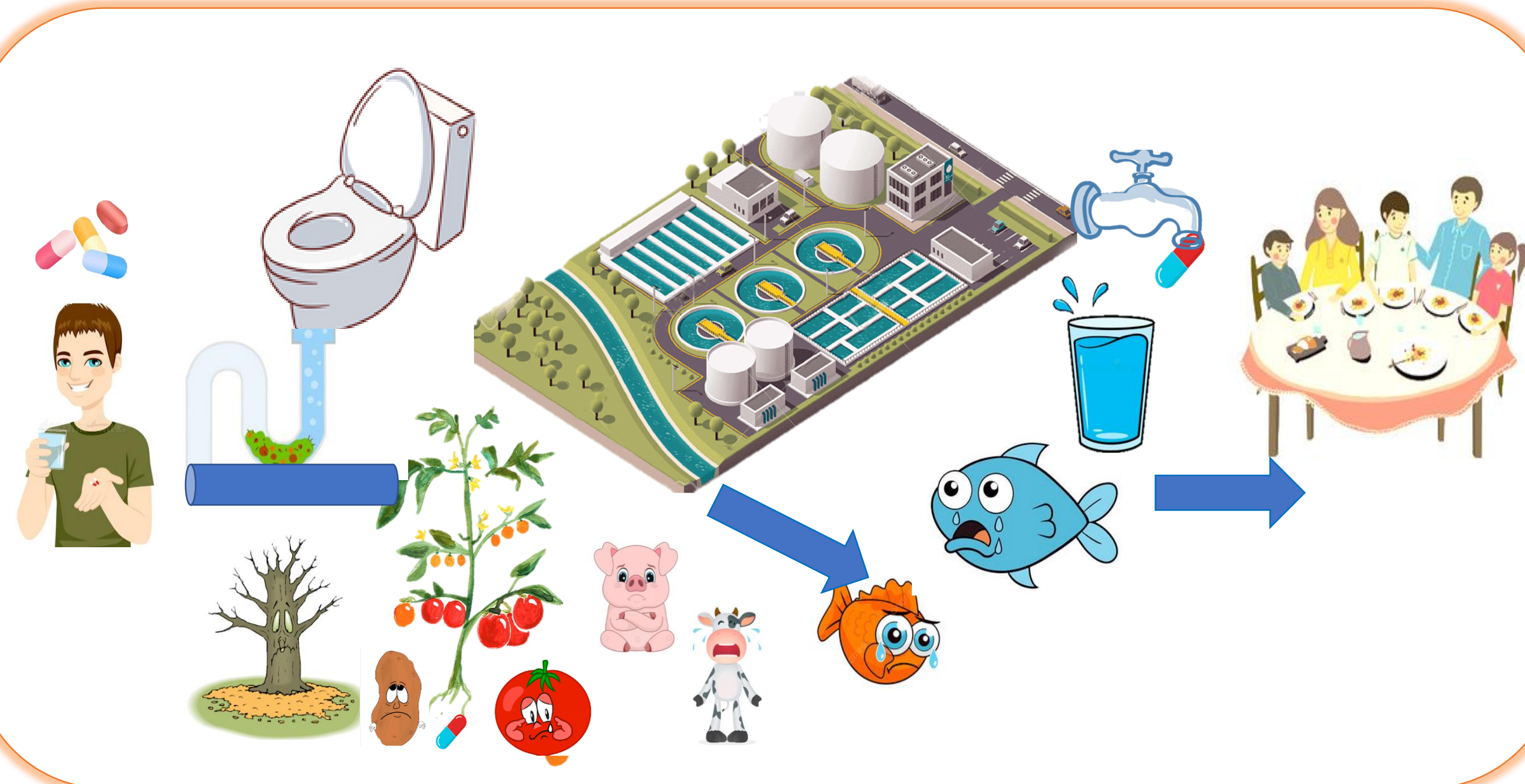
✓ This necessitates a comprehensive understanding of the occurrence, concentration levels, and spatiotemporal distribution of these compounds in aquatic environments, as well as the development and implementation of effective, long-term monitoring strategies to ensure accurate assessment and management of their presence in water systems.

✓ In this context, high-resolution mass spectrometry (HRMS) offers full-spectrum acquisition and represents a promising and powerful technique for screening different classes of pharmaceuticals in water resources, enabling target, suspect, and unknown screening approaches.

SAMPLING

- Water samples were collected from multiple locations along the Great Bačka Canal to capture spatial variability and assess the distribution of pharmaceutical contaminants across different segments of the waterway.
- The selected surface water recipients within the Great Bačka Canal differed in hydrological characteristics, particularly in water flow rates, resulting in varying degrees of dilution of wastewater-derived compounds.
- Additionally, a total of 40 water samples were collected from sites characterized by varying sizes of nearby settlements and differing intensities of industrial activities, which are expected to influence the concentration and composition of pharmaceutical contaminants

THE ROUTE OF PILL IN THE ENVIRONMENT



ECOLOGICAL RISK ASSESSMENT

Environmental risk assessment (ERA) is an essential process aimed at safeguarding our ecosystems from potential harm caused by medicines. ERA was determined by calculating risk quotient (RQ):

$$RQ = \frac{MEC}{PNEC}$$

where: MEC is maximum measured environmental concentration, PNEC is predicted no effect concentrations and depends on the available toxicological data (<https://www.normannetwork.com/nds/ecotox/lowestPnecsIndex.php>)

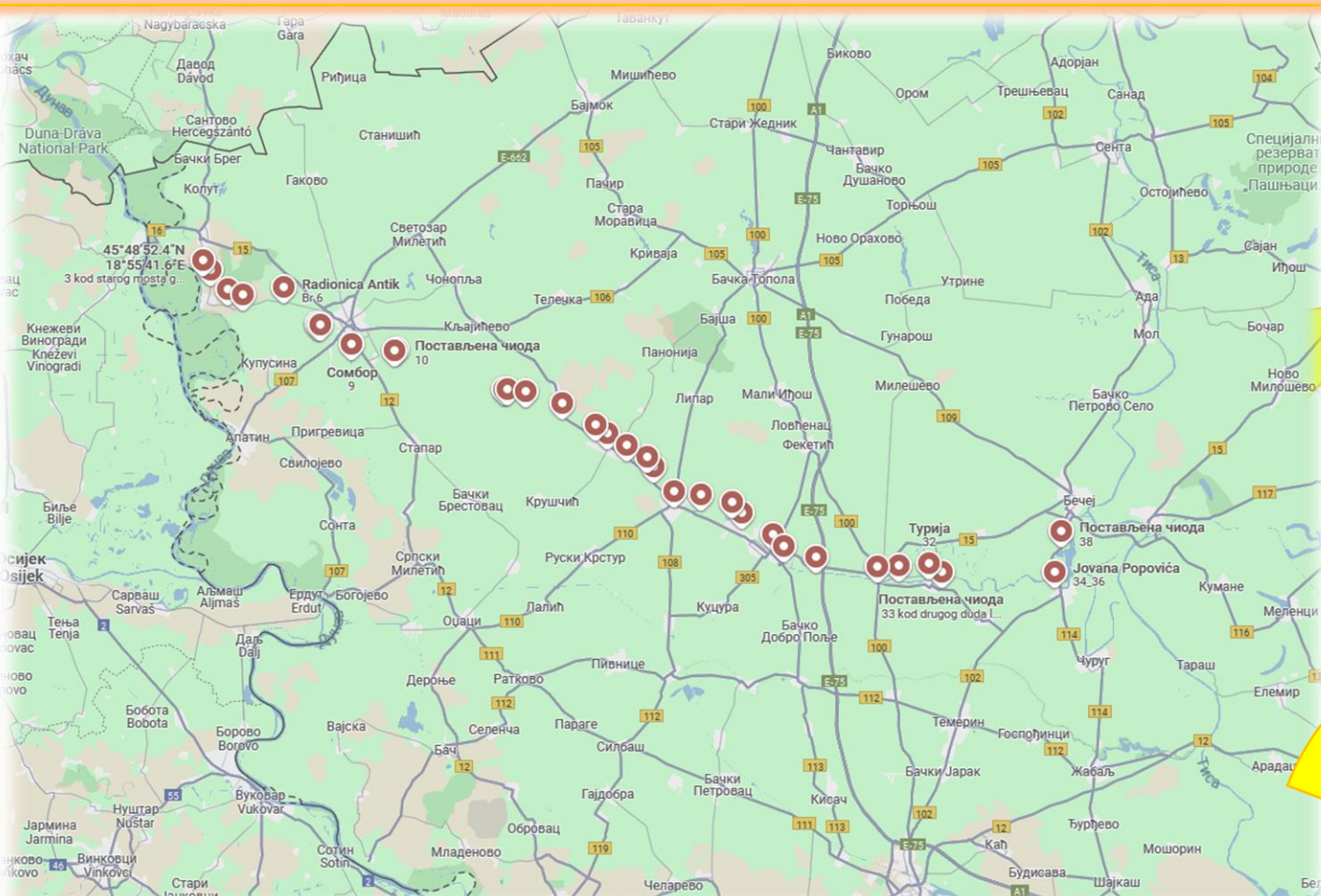
The RQs are classified into three risk levels: values below 0.1 indicate a low risk; 0.1 < RQ < 1 represents a medium risk; and RQ above 1 reveals a high risk and high potential for adverse effects.



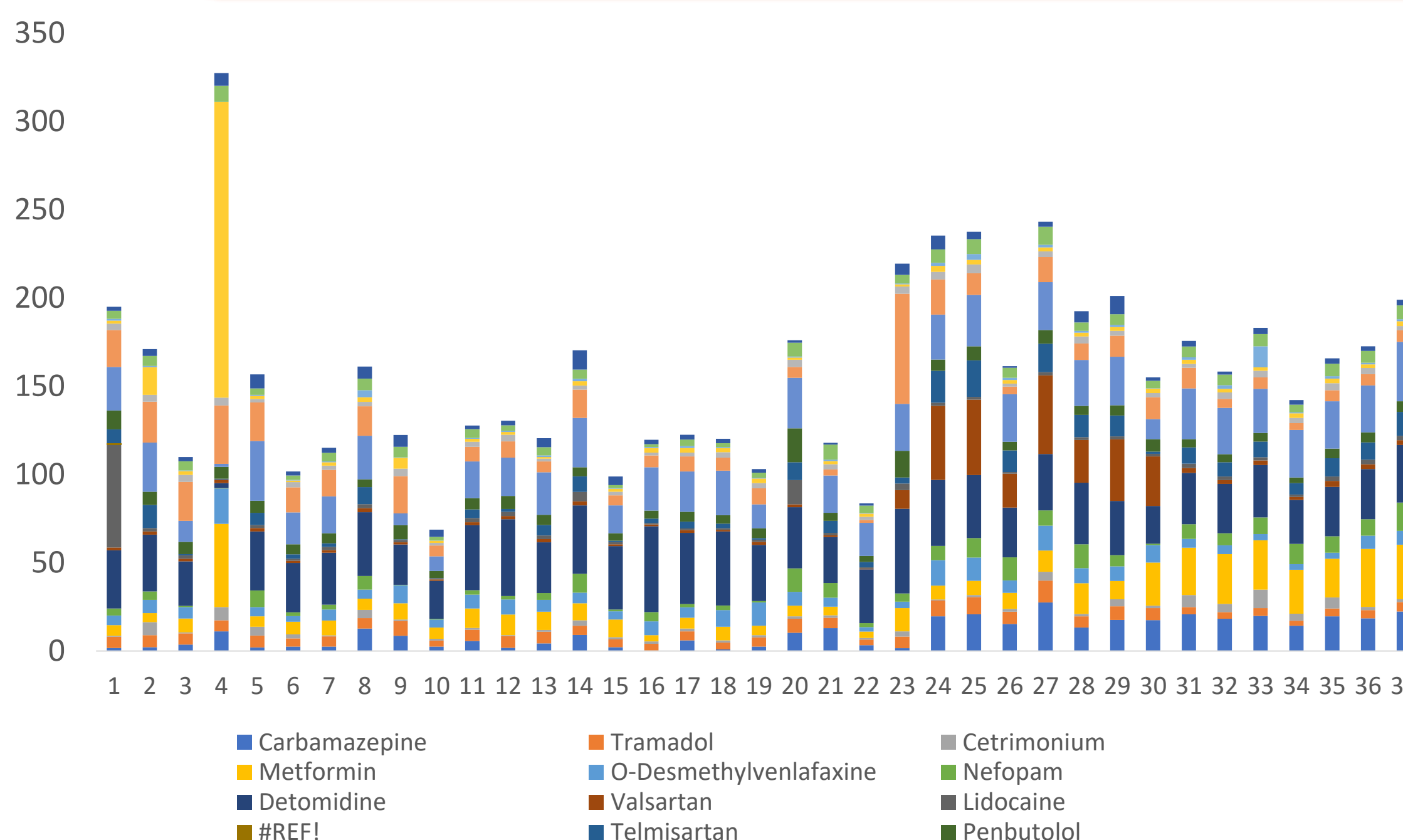
CONCLUSION

- This study investigated the occurrence of 116 PhACs of a wide scope of polarities and physical-chemical properties in surface water sampled from the Great Bačka Canal.
- A total of 18 PhACs were detected in the surface water at the selected sampling sites and their median concentrations ranged from 0.07 (2',2'-Difluorodeoxyuridine) to 167.4 ng/L (valpromide).
- The concentrations of the largest number of detected compounds were in the median range from 1 to 100 ng/L.
- The highest concentrations found in the analyzed surface water were for valpromide (167.4 ng/L), N-desmethyltramadol (62.30 ng/L), and lidocaine (58.03 ng/L).
- The cumulative risk assessment was calculated as the sum of the RQs so-called "cocktail risks". To better explain the risk levels, the RQs are classified into three risk levels: values below 0.1 indicate a low risk; 0.1 < RQ < 1 represents a medium risk; and RQ above 1 reveals a high risk. Regarding RQs for surface water samples collected for each sampling location, values were above 1, indicating environmental risks associated with the occurrence of PhACs were high.

STUDY AREA

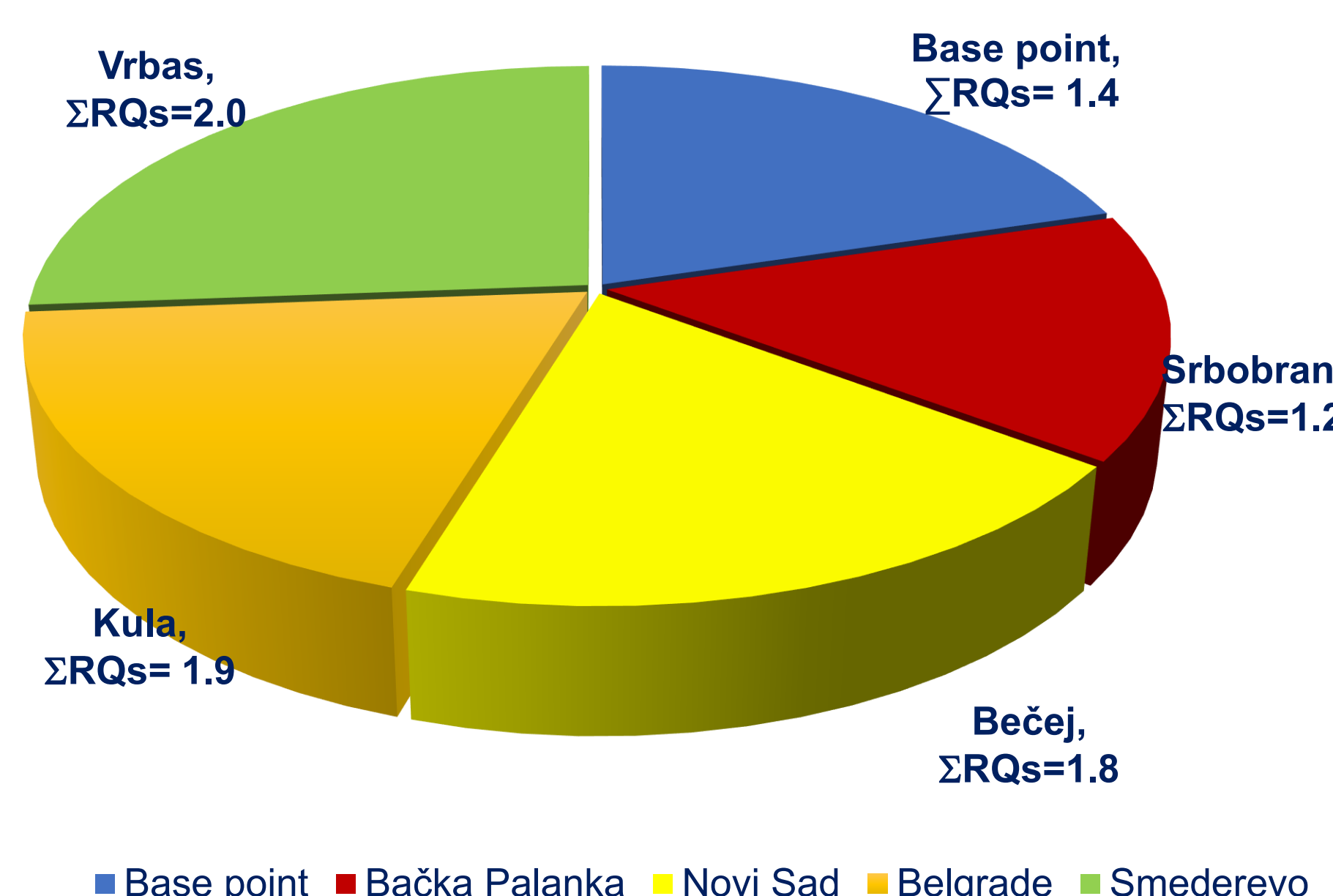


Map of sampling locations



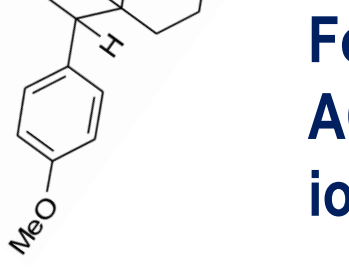
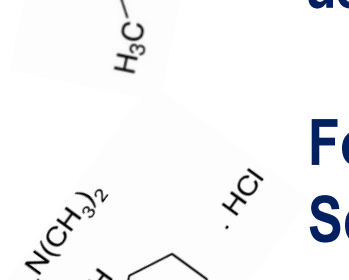
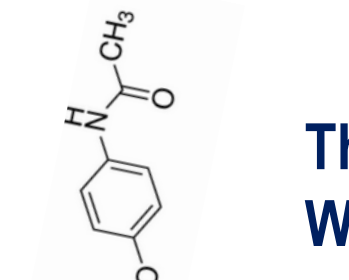
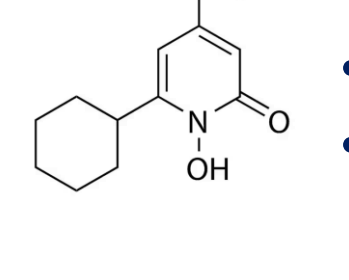
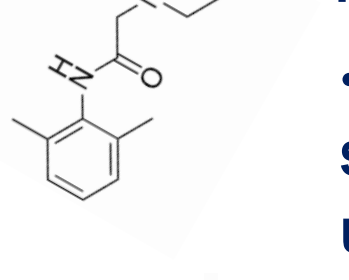
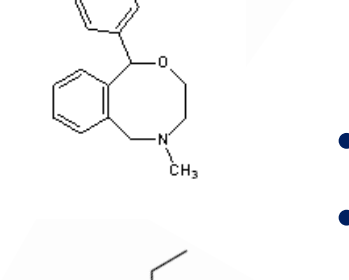
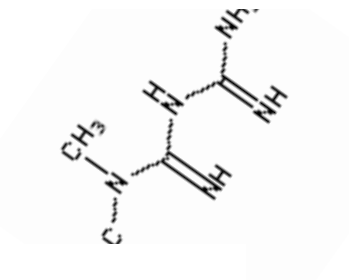
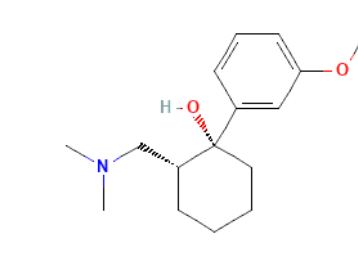
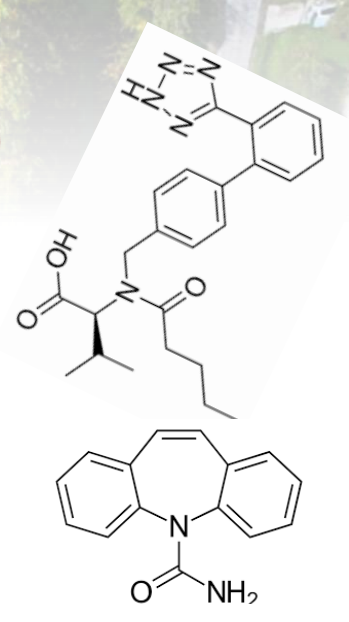
Cumulative concentrations (ng/L) quantified in the studied sampling points

Risk quotient (RQ) calculated for each town



DETECTED COMPOUNDS

Compound name	Class
Valsartan	angiotensin
Carbamazepine	anticonvulsant
Tramadol	pain medication
Cetrimeronium	antiseptic
Metformin	biguanides
O-Desmethylvenlafaxine	antidepressant
Nefopam	painkiller
Detomidine	sedative
Lidocaine	anesthetic
Telmisartan	angiotensin
Penbutolol	beta blockers
N-Desmethyltramadol	pain medication
Ciclopirox	antifungals
Valpromide	mood-stabilizer
2',2'-Difluorodeoxyuridine	anticancer
Neostigmine	myasthenia gravis
Phenacetin	pain-relieving
Venlafaxine	antidepressant



SAMPLE PREPARATION

•500 ml of surface water

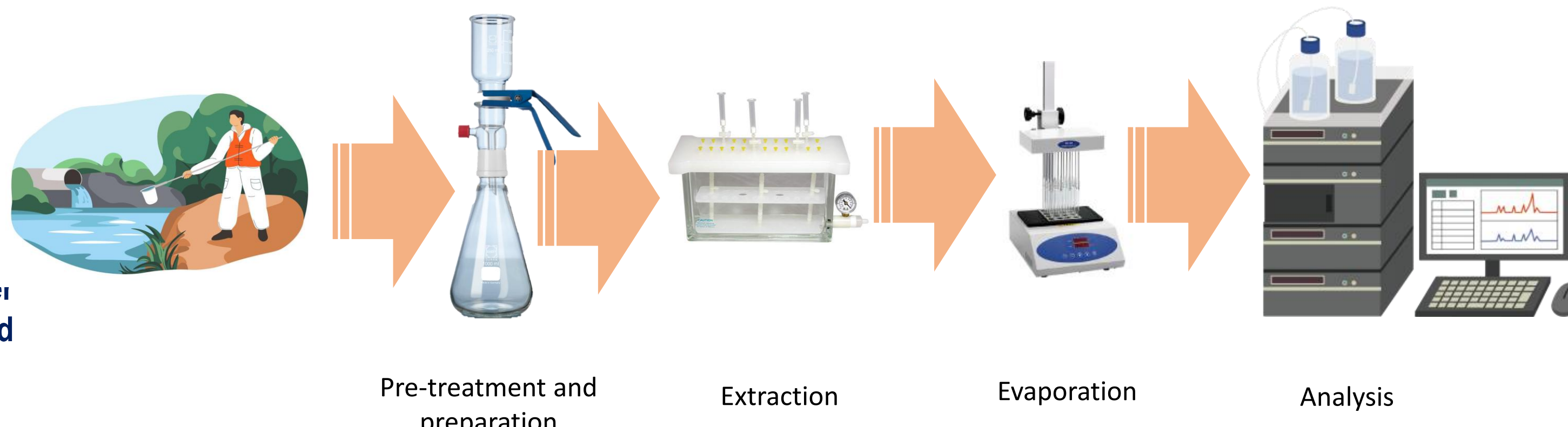
- Filtration through a glass microfiber filter (GF/F)
- Preconditioning: 4 mL 0.1% ammonium hydroxide in methanol followed by 4 mL methanol and 4 mL water.
- Washing: 4 mL of water; 4 mL ammonium acetate buffer, solution (pH 4), and 20 % methanol in water and then dried under vacuum for 30 min before elution
- Elution: 4 mL of 0.1 % ammonium hydroxide in methanol
- Evaporation: to dryness under a gentle stream of nitrogen
- Reconstitution: in 500 µL 40/60 methanol/water (v/v)

INSTRUMENTAL ANALYSIS

The targeted contaminants were separated using ultra high-performance liquid chromatography in a Waters Acquity HSS T3 (C18) column (100 × 2.1 mm i.d., 1.8 µm particle size) thermostated at 40 °C using a Waters ACQUITY UHPLC system (Waters, Milford, MA).

For the detection, a Q-Exactive Orbitrap mass spectrometer (Thermo-Fisher Scientific, Germany) equipped with heated electrospray ionization (HESI) was used.

For the positive electrospray ionization (ESI+), the mobile phases used were ACN and 5 mM AcNH₄ + 0.1% FA in water, while for the negative electrospray ionization (ESI-) mode ACN and 2 mM NH₄F in water were used.



Q-Exactive Orbitrap

H-ESI Parameters	
Spray voltage (kV)	3.75 (+) -3.25 (-)
Capillary T°	360
Heater T°	320
Sheath gas	40
Auxiliary gas flow	5
Sweep gas	0