Target and suspect screening of 4,777 per- and polyfluoroalkyl substances (PFASs) in river water, wastewater, groundwater and biota samples in the Danube River Basin

Kelsey Ng[1,2*], Nikiforos Alygizakis[1,3], Andreas Androulakakis[3], Aikaterini Galani[3], Reza Aalizadeh[3], Nikolaos S Thomaidis[3], Jaroslav Slobodnik[1]

[1] Environmental Institute, Okružná 784/42, 97241 Koš, Slovak Republic

[2] Faculty of Science, Masaryk University, RECETOX, Kamenice 753/5, Building D29, 62500, Brno, Czech Republic

[3] Laboratory of Analytical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece

best chemical risk assessment professionals for maximum ecosystem services benefit

***Presenting author – contact: ng@ei.sk / 527416@muni.cz**

Background

- The Danube provides drinking water to 20 M+ people & key ecosystems to the Danube River Basin (DRB) → it is essential to ensure the water quality
- Anthropogenic activities introduce contaminants to the DRB including PFASs.
- Majority of the previous investigations targeting PFASs in the DRB were performed solely with "conventional" target screening approach, while suspect screening is a powerful complementary tool to reveal novel contaminants.
- Infrastructure on the NORMAN Database System (such as the SLE and DSFP) support the retrospective suspect screening of thousands of PFASs

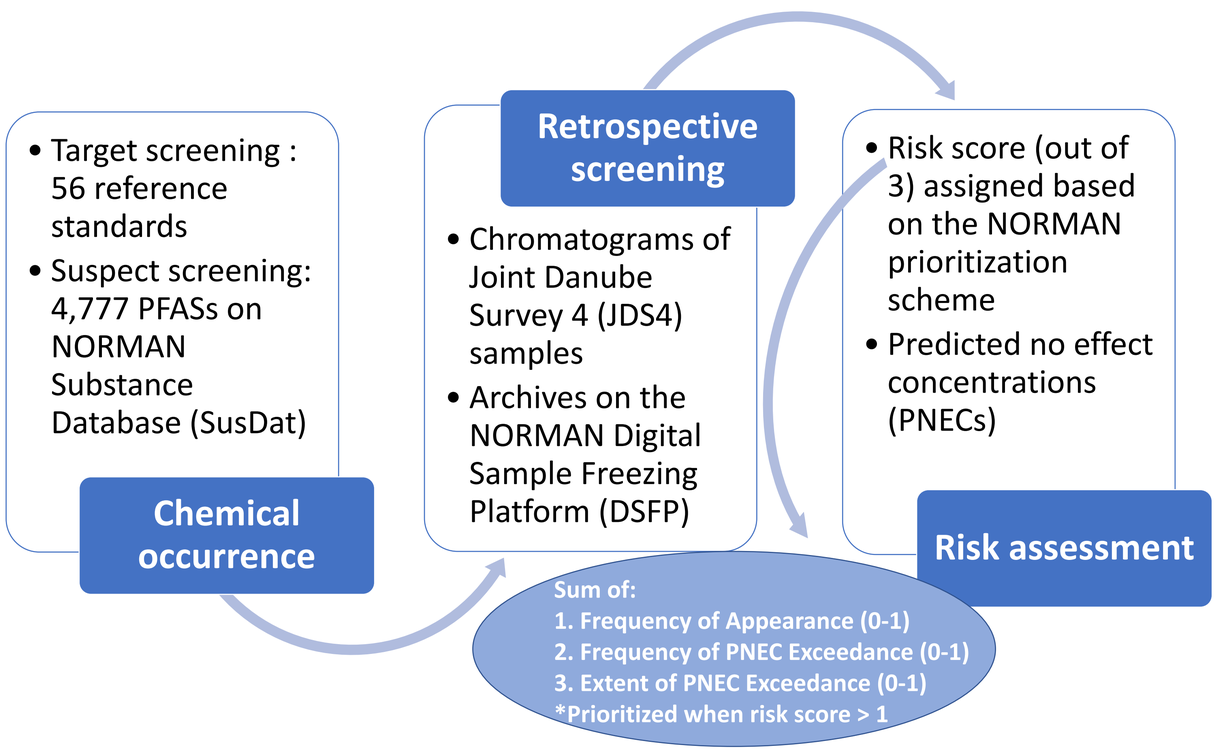
Objectives

To screen: PFASs in the DRB using LC-HRMS and LC-MS/MS (special focus: reveal novel PFASs)

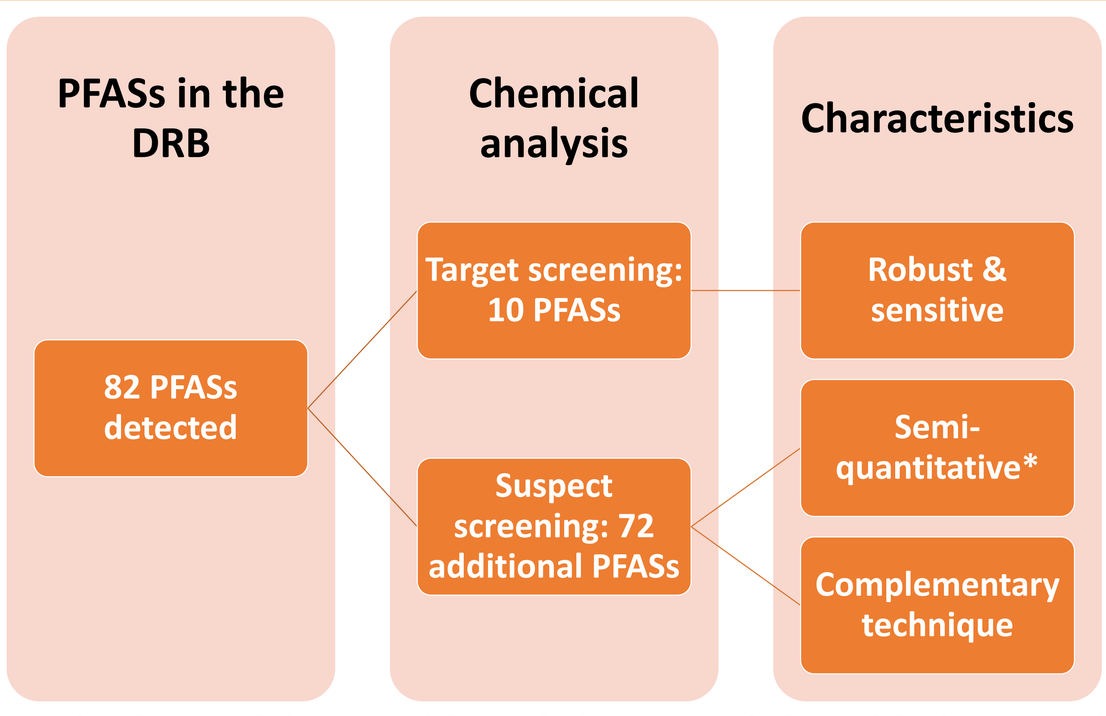
To investigate: distribution of PFASs in the studied matrix (river water, wastewater, groundwater & biota; 95 samples in total)

To characterize: potential threats of PFAS pollution by environmental risk assessment (ERA)

Chemical analysis & ERA



Environmental presence of 82 PFASs in the DRB



*Same order of magnitude for >90% of the 224 findings commonly detected by the 2 approaches

Figure 1. Performance of target & suspect screening in the investigation

Distribution of PFASs in the studied matrices

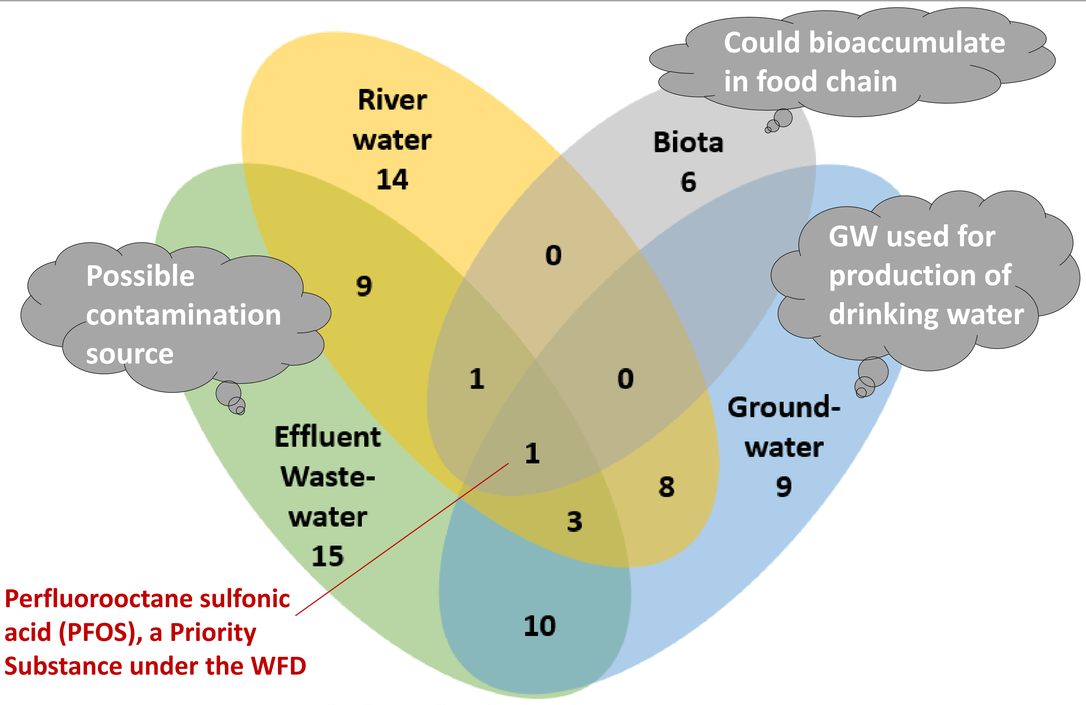
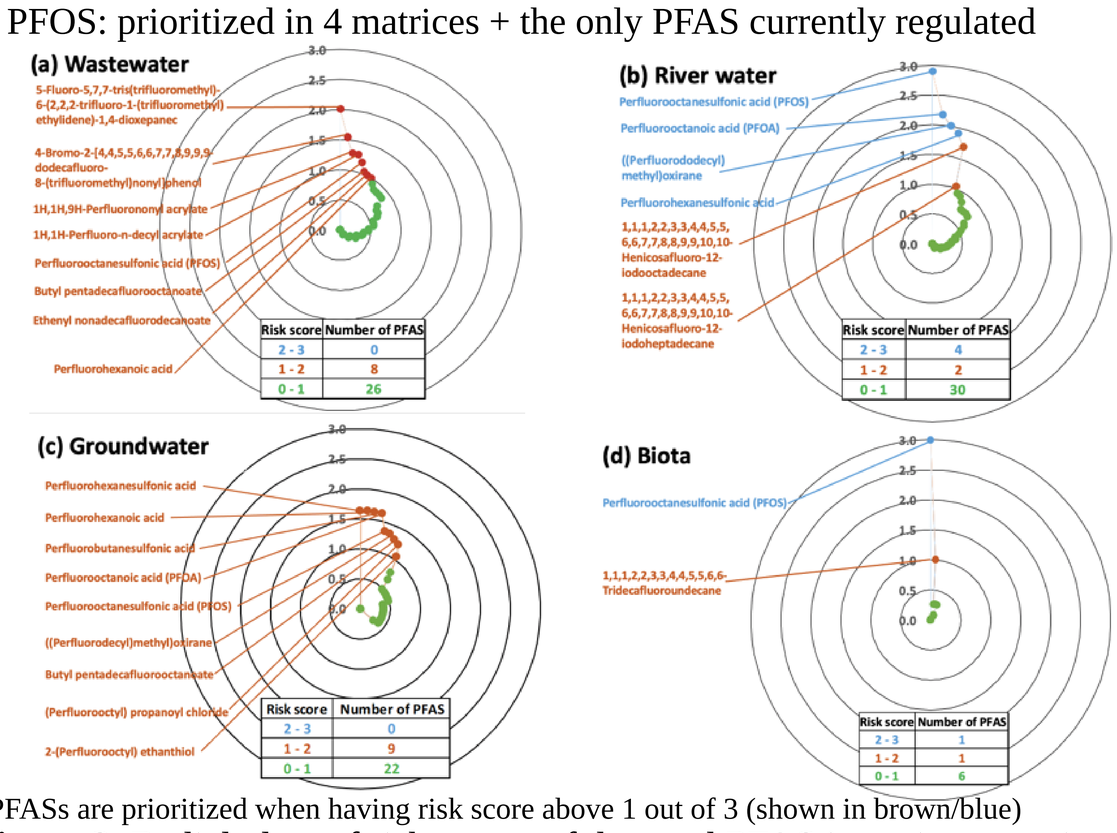


Figure 2. Occurrence of identified PFAS in various matrices

Risk characterization

- 18 PFASs prioritized, of which 13 were detected only by suspect screening
- PFOS: prioritized in 4 matrices + the only PFAS currently regulated



*PFASs are prioritized when having risk score above 1 out of 3 (shown in brown/blue)

Figure 3. Radial plots of risk scores of detected PFAS in various matrices

Discussion & Conclusion

- **82 PFASs** were detected in the **95 DRB environmental samples**, of which **72 were detected only by suspect screening** → suspect screening proven to be a powerful complementary tool to reveal novel PFASs.
- PFASs were detected in biota (fish) and groundwater samples, which could reach human via food chain/drinking water.
- **18 PFASs were ranked** in the ERA following the NORMAN prioritization scheme, of which **17 of them are not currently regulated.**
- It is essential to identify source & fate of PFASs in the DRB and establish **regulatory monitoring of PFASs (especially for prioritized ones).**

Acknowledgement & References

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 859891. This presentation reflects only the authors' view and the European Commission is not responsible for any use that may be made of the information it contains. Special thanks to Dr. Jaroslav Slobodnik and Dr. Nikiforos Alygizakis for supervising the study.

Reference: Ng, K., Alygizakis, N., Androulakakis, A., et al., *Target and suspect screening of 4777 per- and polyfluoroalkyl substances (PFAS) in river water, wastewater, groundwater and biota samples in the Danube River Basin.* J Hazard Mater, 2022. **436**: p. 129276.