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Editorial: Chemometric approach to distribution, source apportionment, ecological and health risk of trace pollutants

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Editorial on the Research Topic
Chemometric approach to distribution, source apportionment, ecological and health risk of trace pollutants

Intensive technological development has led to tremendous pressure on the quality of the environment, which is reflected in its pollution by toxic trace pollutants. The modern approach to studying risks from these pollutants includes the integration of analytical chemistry, environmental science, mathematics, statistics, and toxicology. A dramatic increase in data generated by modern analytical instruments in studies on trace pollutants in the environment imposes a quite complex task to extract meaningful information from these data. Thus, the use of chemometrics became irreplaceable.

Principal component analysis (PCA) (Radomirović et al., 2020; Trujillo-González et al., 2022a), hierarchical cluster analysis (HCA) (Lučić et al., 2022), positive matrix factorization (PMF) (Radomirović et al., 2021), geostatistical analysis (GIS) (Trujillo-González et al., 2022b); (Miletić et al., 2022), Monte Carlo simulation (MCS) (Seyednejad and Ghiasi, 2022), numerical modeling (Wang et al., 2019), machine learning and artificial intelligence modeling (ANN) (Egbueri, 2021; Agbasi and Egbueri, 2022) have been frequently used chemometric methods for trace pollutants data evaluation. Since there is great competitivity or complementarity between these methods, it is common to use several methods together in a single study. Therefore, a comprehensive approach is needed in this area where different research can be incorporated, covering a range of chemometric methods and their combinations for various pollutants in the environment.

This Research Topic addressed recent advances in the application of chemometrics in studies on the occurrence, distribution, and fate of trace pollutants in different media (soil,

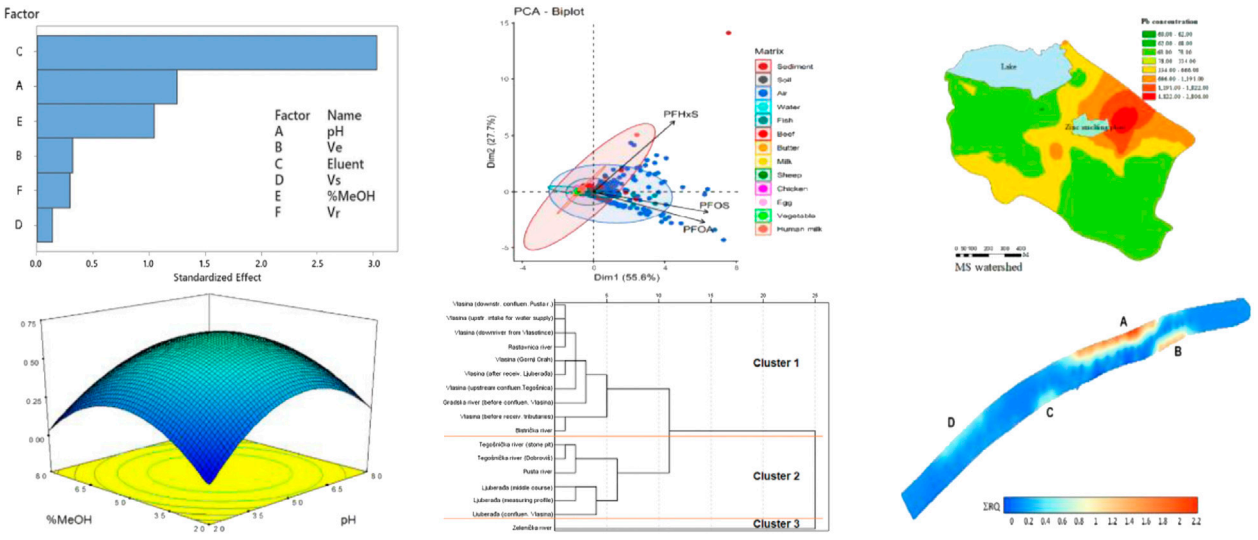

FIGURE 1
Some of the figures from the research topics. **(A)** Pareto chart from the screening Plackett-Burman experimental design. **(B)** Response surface optimization graph. **(C)** PCA-Biplot. **(D)** Dendrogram from HCA. **(E)** GIS map of soil. **(F)** GIS map of water.

air, water, plants, and food). It was focused not only on pattern recognition, classification, and pollution source identification but also on ecological and health risk assessment.

Nine articles after peer review were published in this Research Topic. These articles highlighted a diversity of chemometric methods for the fate of toxic pollutants and their influence on the environment and human health. Figure 1 illustrates how some of the mentioned methods present the data in these articles.

The contamination by toxic trace elements was investigated in several articles. Heavy metals in urban dust and possible ecological and human health risk in six Mexican cities were studied by Aguilera et al. It was found that all studied cities were contaminated, while the highest metal contribution to the potential ecological risk in all the cities was from Pb. Therefore, the importance of identifying the main sources of Pb in cities and seeking mitigation strategies to reduce its possible adverse effects was highlighted.

Yu et al. investigated the superposition effects of atmospheric deposition from zinc smelting on soil heavy metal pollution under geochemical anomaly. The results showed much higher concentrations of heavy metals in the atmospheric deposition area where a zinc smelting plant was situated than those in the control area with the local background values. PCA reflected more diversified pollution sources, while the GIS distribution of soil heavy metals indicated that the content of heavy metals in soil was highly dependent on the location of zinc smelting.

A case study in Peninsular Malaysia on the health and ecological risk of Sb and As in the vegetable *Centella asiatica*, topsoils, and mangrove sediments was conducted by Yap et al. The findings indicated that 56% of the topsoils with As hazard index (HI) values for children exceeded one. The ingestion pathway contributed almost all the As total HI values. Furthermore, a high ecological risk of As and carcinogenic health risk of As in the topsoils and mangrove sediments were evident, with the HI values in children being higher than those in adults. Anthropogenic sources of Sb and As originated from land-based activities before reaching the mangrove near the coast were apportioned.

An integrated approach in the assessment of the Vlasina river system pollution by toxic elements was used by Sakan et al. The water and sediments of rivers in the Vlasina region (Serbia) were analyzed to assess the current state of pollution with toxic elements. No significant spatial variability of potentially toxic elements in water and sediments was observed. The positive correlations between most of the examined elements in sediments indicated their dominant geochemical origin. It was found no notable pollution in the water and sediments in the Vlasina region.

Zhang et al. investigated bioaccumulation and assessed the risk of potentially toxic elements (PTEs) in the soil-rice system in a karst area (Southwest China). The results revealed that weathering of parent rocks and alluvial deposits was the major source of heavy metals in soils, while fossil fuel combustion and agricultural activities also contribute to the accumulation of soil PTE. The high excessive rate of Cd and Pb could be attributed to their high bioaccumulation factor and high content in the soil. At the same time, residents may be exposed to As and Cd through rice consumption. The average targeted hazard quotient values (THQ) of PTE for the rice samples decreased in the order of

As > Cd > Cr > Cu > Zn > Pb > Hg, and the degree of a health risk it posed to the population was Children > Female > Male. Therefore, health risks caused by excessive consumption of wild heavy metal-enriched rice should be avoided.

A consumption risk from trace metal residues in swimming warrior crab (*Callinectes bellicosus*) has been studied by Castro-Elenes et al. They found a high contamination level of trace metals in the edible tissue of crabs, resulting from a constant discharge of these pollutants to the lagoon from the agricultural and aquaculture activities after irrigation or wastewater drainage. These trace metal residues are being bioaccumulated in the edible tissues of the crab due to its feeding habits, resulting in carcinogenic and non-carcinogenic health risks if its consumption is high.

Bacterial Cd immobilization activity (CIA) in cacao-growing soils from Colombia has been studied by Bravo. He measured CIA by Cd-tolerant bacteria (CdtB) using isothermal microcalorimetry (IMC). A Pearson correlation analysis was made between kinetical growth parameters and thermodynamic data, while PCA of CdtB cadA gene copies, soil pH, and soil organic matter indicated the effect of CdtB in Cd translocation. The research importance of his work was the use of combined tools for quantitative IMC measurements to identify and assess Cd metabolic capacities of CdtB populations in soil, *in situ*.

In the study of Fiedler et al., a multivariate evaluation of perfluoroalkyl substances (PFAS) in environmental samples, including air, water, sediment, soil, food samples comprising fish, meat (beef, sheep, chicken), egg, butter, and milk as well as human milk samples have been done. This assessment of PFAS in abiotic and biota samples showed that perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) dominated the scale and the pattern in all matrices.

Chemometric optimization of the solid-phase extraction (SPE) procedure used in the extraction of eleven ultraviolet filters (UVFs) from urban lake water was reported by Lukić et al. They applied the Plackett-Burman design, the Box-Behnken design, and Derrindzer desirability function to screen and optimize six SPE variables. The optimized SPE was then implemented to prepare the water samples prior to liquid chromatography-tandem mass spectrometry (LC-MS/MS) measurements. Finally, the Monte Carlo simulation of environmental risks and sensitivity analysis were performed, revealing a safety concern due to UVFs in the long term. Geostatistical mapping of the risk quotient in a lake showed that its was highly dependent on recreational activities.

In conclusion, combining chemometric techniques and risk indices is helpful in assessing environmental pollution status. Potentially toxic elements are still the most studied pollutants. Among the organic trace pollutants, emerging organic contaminants are of particular safety concern. Future works are expected to address new contaminants, lower concentrations, larger datasets, and new approaches to health risk assessment.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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