Investigation of the presence and removal of emerging contaminants at various stages of industrial wastewater treatment

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Nowadays, an ever-increasing number of pollutants are entering the environment due to various human activities, posing serious risks to human health and ecosystems. In the past, global research primarily focused on the study of priority pollutants, due to their known persistent, bioaccumulative, and toxic (PBT) properties. However, priority pollutants represent only the "tip of the iceberg," as many other compounds have neither been legislated nor sufficiently studied [1].

In recent decades, the development of new, more sensitive analytical techniques has revealed the presence of many other potentially hazardous substances known as "emerging contaminants." Emerging contaminants are organic compounds that are not included in routine monitoring or existing legislation [1]. Nonetheless, concern about them is growing due to their frequent detection in the environment and the often-unknown threats they pose. Industrial activities are one of the main sources of these pollutants, and the disposal of industrial wastewater poses a significant threat to ecosystems and human health due to its high toxicity and complex composition [2].

Taking all the above into account, the present study aims to develop reliable and effective analytical workflows for the determination of emerging contaminants and to investigate their presence and removal at various stages of industrial wastewater treatment.

For this purpose, the technique of choice was ultra-high-performance liquid chromatography coupled with ion mobility spectrometry and high-resolution mass spectrometry (UHPLC-TIMS-QToF-MS). Specifically, high-resolution mass spectrometry was used for targeted analysis across a wide range of compounds (wide-scope target screening), as it offers the capability to identify numerous compounds that differ minimally in their mass. Furthermore, an internal database containing over 2,400 emerging pollutants, priority pollutants, and their biotransformation products was utilized for data processing.

The identification of the compounds was conducted using strict parameters related to mass error, retention time shifts, isotopic patterns, and the presence of qualifier ions. Additionally, the incorporation of ion mobility spectrometry allows for the inclusion of collision cross-section (CCS) as an additional orthogonal identification parameter, which often resolves the issue of separating isomers and isobars. Filtering based on time and ion mobility also provides cleaner MS and MS/MS spectra.

Finally, the aforementioned technique was applied to samples of industrial wastewater, which were pretreated using a generic sample preparation protocol. Numerous compounds from various categories were detected, including personal care products, plant protection products, and pharmaceutical compounds.

References:

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