Assessing Efficiency and Byproducts Formation of Several AOP Techniques for Potable Water Reuse

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Introduction & Objective

Context and Background
- Water scarcity due to climate change and the increasing water demand leads a growing number of large cities worldwide to consider potable water reuse.
- Most potable water reuse strategies involve advanced oxidation processes (AOPs) for the attenuation of trace organic contaminants.
- While water treatment processes are often evaluated by monitoring the concentration of selected contaminants, little is known about the fate of unknowns and by-products.

Objective
- Use QTOF analysis and sample profiling to assess the attenuation of known and unknown contaminants by AOPs along with the formation of by-products.

Sample Preparation & Analysis

Sample Preparation
- Filtration on GFF filter
- Solid Phase Extraction Dionex Autotrace HLB cartridges (Waters)
- Sample volume: 375 mL
- Final Extract: 0.5 mL

LC-QTOF Analysis
- Liquid chromatography Agilent 1290 series Zorbax C18 column 3 μL injection (triplicate)
- Mobile phase H2O/O2/H3N

Data Processing
- MassHunter software
- Extraction of chromatograms
- Extraction of molecular features
- Mass Profiler Professional software
- Filtration of molecular features
- Principal Component Analysis
- Visualization of sample profile

Sample Profiling & Clustering

Chromatograms & Extraction of Molecular Features
- Most of the chromatograms appeared similar.
- Close to 1000 molecular features extracted in each chromatogram.

Software essential for further data processing.

Principal Component Analysis

PCA Plot for Different Ozone Doses
- QTOF analysis showed AOPs attenuate multiple unknowns beyond target organic compounds commonly monitored.
- Advanced data processing with Mass Profiler Professional allows the clustering of compounds with the same behavior during water treatment.
- Compounds with similar behavior could be used as indicator in order to limit the amount of target analytes for the assessment of treatment efficiency.
- Further sampling campaigns are required to confirm the identification of robust clusters around contaminants routinely analyzed.

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