

# **Fate and distribution of emerging contaminants in the marine ecosystem, following extreme climate change induced storm events at Aegean Sea, Greece, Eastern Mediterranean, utilizing the technique of LC-VIP-HESI-TIMS-HRMS**

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Emerging contaminants, such as plant protection products, pharmaceuticals and PFASs, coming from various human activities, often end up in the marine environment and are distributed in different compartments, namely sea water and sediments.

In Thessaly, Greece, sequential storm events “Daniel” and “Elias” rained down 1.5 million tons of water per square kilometer in the area of Pagasitikos Gulf (Aegean Sea, Eastern Mediterranean) each day the phenomena were in effect, during the fall of 2023. Such major storm events linked with climate change can increase the number of pollutants ending up in the aquatic ecosystem.

To study the distribution and fate of various emerging contaminants and their transformation products, 34 seawater and 27 sediment samples were collected from the marine area about twenty days after the last storm event. To extract as many contaminants as possible, generic sample preparation protocols were applied utilizing mixed-mode Solid Phase Extraction and Ultrasonic Assisted Extraction. The analytes were separated via Liquid Chromatography linked to a hybrid Trapped Ion Mobility Spectrometer coupled to a High-Resolution Mass Spectrometer (TIMS-HRMS). The presence of approximately 2,500 chemicals was investigated, by implementing wide-scope targeted workflows.

Results indicated the presence of numerous pharmaceuticals, plant protection products and PFASs. Various pharmaceuticals with concentrations up to 795 ng/L in seawater and 29.0 µg/g in sediments were determined, probably due to sewage treatment plants’ overflowing caused by the floods. Their distribution between seawater and sediments was related to their water solubility and particulate material formation, as seems to be the case for quinolone and sulfonamide antibiotics, which were detected only in sediments.

Regarding plant protection products, numerous compounds were detected in areas close to river estuaries (total of 197 ng/L in seawater). Some of them, like Azoxystrobin were distributed in both compartments, polar compounds, like Atrazine along

with its transformation products were only found in seawater, while less polar pesticides were solely detected in sediments.

PFASs were detected in every sample analyzed, with 6:2 Fluorotelomer sulfonic acid surpassing every other PFAS in terms of concentration, ranging from <LOQ levels to 815 ng/L in seawater and 0.511 µg/L to 26.4 µg/g in sediments.