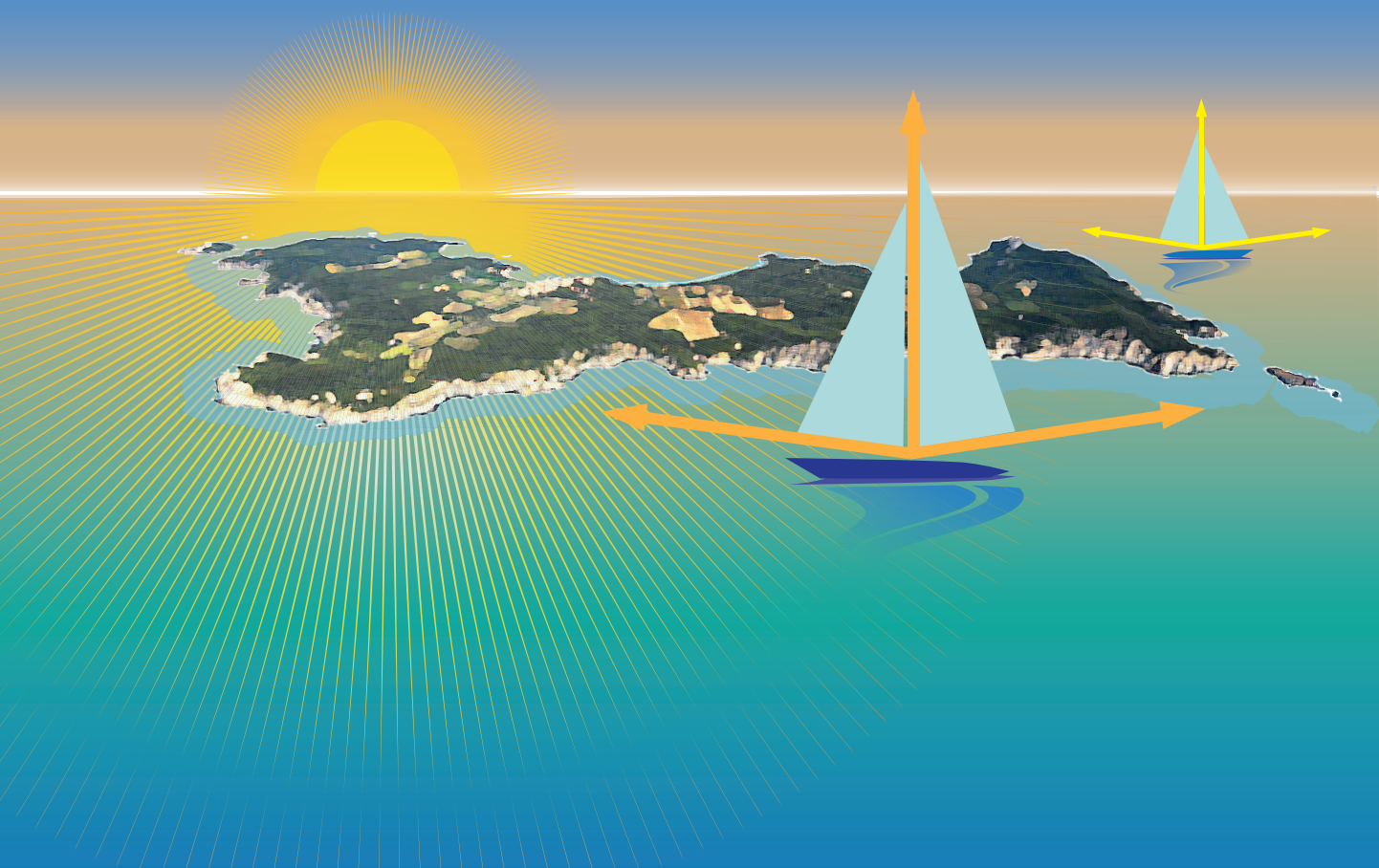


XII

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Mapping Emerging Organic Contaminants in wastewater, superficial and sub-superficial water by untargeted uHPLC-HRMS

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Emerging organic contaminants (EOCs) can be of both natural and synthetic origin, and include a wide range of industrial, agricultural, pharmaceutical and consumer products, such as plasticisers, pesticides, fertilisers, antibiotics, hormones, parabens and PFAS (perfluoroalkyl substances) and their metabolites [1]. Their poor biodegradability and tendency to bioaccumulate in environmental matrices makes them potentially hazardous for causing health damage in the long term, see [2] for a first list of concern. This study aims at obtaining a first mapping of EOCs in different kind of water samples, such as surface water (three sampling sites) and groundwater (six sampling sites), since these are vital resources for water supply for drinking, agricultural and industrial purposes, as well as wastewater (six sites sampled at entrance and exit of a wastewater treatment plants, WWTP). In fact, numerous studies have shown a correlation between the presence of these contaminants and treated water from conventional municipal, WWTPs [3], considering that WWTPs were not originally designed to remove these types of pollutants. An untargeted approach based on uHPLC (using a ZIC-cHILIC stationary phase) coupled to high resolution mass spectrometry (by using Orbitrap Q-Exactive) was carried out to explore the presence of EOCs and for some of them estimate the content by using reference standards. EOCs were sampled and preconcentrated by solid phase extraction (by testing different SPE cartridges). The data arising from uHPLC-HRMS are very complex and we resort to Multivariate Curve Resolution – Region of Interest (ROI-MCR) method [4], taking care of properly optimizing the hyperparameters, followed by further multivariate data analysis to compare the different samples sites.

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