Environmental forensics in seawater coupling a divinylbenzene passive sampling device and high resolution mass spectrometry for the screening of micropollutants

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Abstract (max 2500 characters with space)

Environmental analysis encouters analytical difficulties such as fluctuating concentrations (due to variation in space and time), complex mixtures of micropollutants, and different transformation products of the same emerging substances (due to environmental conditions). Combining passive sampling techniques with the analysis of ultra-high-performance liquid chromatograpy high resolution mass spectrometry (UHPLC-HRMS) will improve environmental metrology. Next, passive samplers accumulate compounds during exposure, which improves the detection of organic micropollutants.

The aim of this study was to sequester polar to non-polar emerging organic micropollutants in the marine environment by using a divinylbenzene (DVB) passive sampler coupled by two in-house validated UHPLC-HMRS methods. Comparing the two UHPLC-HRMS methods, eliminates the analytical preconceptions of the organic micropollutants' physico-chemical preferences, caused by sample treatment and chromatographic and ionization conditions. The analyses of the samples were processed in three approaches, i.e. target, suspect and non-target screening. The target screening was based on the preselection of 145 micropollutants in the UHPLC-HRMS method, including pharmaceuticals, personal care products, pesticides, natural and synthetic hormones. The suspect screening, using a scientific database compiled by scientific literature data, enables the identification of 380 micropollutants, including the same therapeutic classes as the target analysis. The non-target screening combines multi-variate analysis and online databases for the identification of unknown micropollutants. The DVB passive sampler coupled to UHPLC-HRMS methods has shown promising results for target, suspect and non-target screening. The three screening approaches have contributed to a specific molecular print for the sites in the marine environment.

The future perspective is the continuous improvement of the molecular fingerprinting. This can be realised by deploying and monitoring the passive samplers during different periods, and comparing them with previous molecular data. Thereby, analysing the DVB passive samplers with other UHPLC-HRMS methods will enable other new target, suspect and non-target compounds. Finally, this work is an important step towards the improvement of environmental monitoring and related programs.