An Omics Approach Towards Identification of Unknown Emerging Pollutants in Marine Waters

Huysman Steve[1], Vanryckeghem Francis[2], Demeestere Kristof[2] and Vanhaecke Lynn[1,3]
[1] Department of Veterinary Public Health and Food Safety, Ghent University, Ghent, Belgium
[2] Department of Green Chemistry and Technology, Ghent, Belgium
[3] Institute for Global Food Security, School of Biological Sciences, Queen's University, Belfast, United Kingdom
E-mail: Steve.Huysman@UGent.be and Lynn.Vanhaecke@UGent.be

The potential prevalence of emerging organic micropollutants in the aquatic environment has become a significant risk for public and ecological health, which is stressed by different regulatory bodies. Despite this, legislation so far mainly focuses on a few priority pollutants, thereby missing a substantial fraction of the known and unknown compounds occurring in water. Hence, the prevalence and identity of most compounds remains unexplored. Therefore, this study presents a novel analytical strategy for elucidating structurally related emerging organic pollutants in the aquatic environment. In-house developed and validated UHPLC-HR-Q-Orbitrap-MS methods targeting 70 steroids (*Huysman et al., 2017*) and 27 plasticizers (*Huysman et al., 2019)* were used to enable the detection of 1292 unique unknown emerging organic pollutants in 24 seawater samples (obtained from the Belgian part of the North Sea). To elucidate typical fragmentation profiles and identify characteristic fragments of the above-mentioned chemical pollutants, the target standards were respectively fragmented at 35 and 20 eV. As a result, typical fragmentation profiles were obtained for the steroids and plasticizers. The generated fragments of the unknowns were screened – using a newly written Python code – on their agreement with characteristic fragments and neutral losses obtained from the target standards. In total, 13% (n=173) of the unknowns present in water could be tentatively identified, i.e. 125 steroids, 21 alkylphenols and 27 phthalates, at a confidence level of Tier 3. Finally, during untargeted screening of seawater samples, all target analytes were successfully detected, confirming that fragmentation occurred also in a salty matrix.