

TARGETED, SUSPECTED & NON-TARGET SCREENING WITH HIGH RESOLUTION MASS SPECTROMETRY IN THE MARINE ENVIRONMENT: READY TO GO?

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Introduction

Many organic micropollutants, such as pharmaceuticals, pesticides, **natural and synthetic steroids** have received special attention because of their omnipresence in the environment. Frequently, these compounds find their way to the environment as **water pollutants**, whether or not metabolised or degraded, resulting in some constraints towards environmental monitoring. While triple quadrupole analysers currently enable only a predefined list of compounds in samples, high resolution mass spectrometry (**HRMS**) make it possible to detect a **virtually unlimited** number of compounds in a single run without preselection. Therefore, an in-house validated UHPLC-HRMS method was used for screening the marine environment on steroidal EDCs. This study included the quantification of 70 **targeted** steroidal EDCs, and on top of that the **suspected** screening of 225 EDCs and a **virtually unlimited** number of unknown compounds.

Objectives

Challenges:

- Micropollutants present at **sub ppb-concentrations**
- Different biotic and abiotic processes result in a wide range of **known** and **unknown** transformation products of the micropollutants

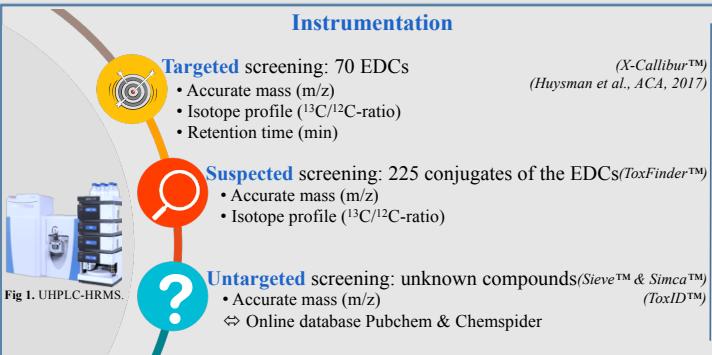


Goals:

- Evaluating an **environmental omics** approach using HRMS
- **Screening** the marine environment on steroidal EDCs
- Performing 3 analytical approaches: targeted, suspected, and untargeted analysis
- Composing a **relevant suspected database**
- Assessing the impact on the marine environment, i.e. toxicity and **potential harm**

Materials & Methods

Instrumentation



Sampling, pre-treatment & extraction

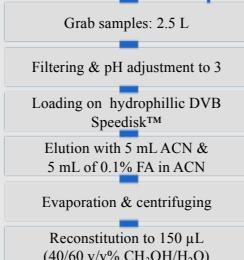
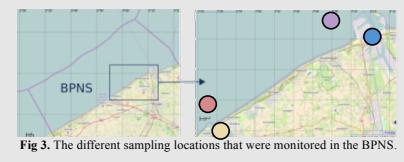
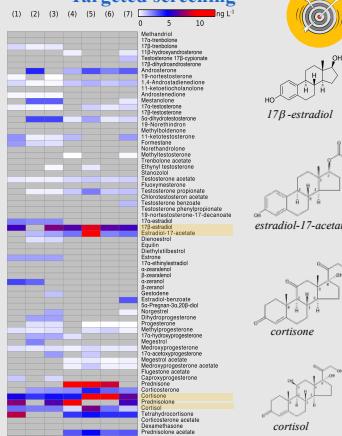


Fig 2. Optimised extraction protocol for grab samples obtained from the marine environment.

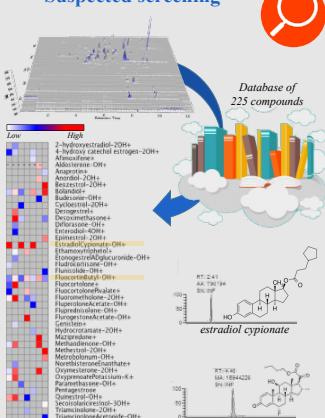


Results

Targeted screening



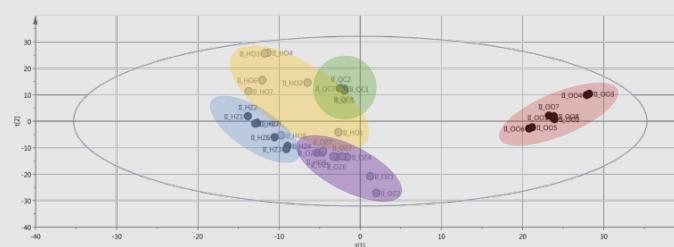
Suspected screening



Untargeted screening

Multi-variate analysis

- Scaling: pareto
- Transformation: log
- Compound Intensities $> 10^6$



Conclusion

The marine environment was successfully screened using an environmental omics approach:

- **Targeted** screening: 43 different steroidal EDCs were quantified
- **Suspected** screening: 44 unique suspected EDCs were detected
- **Untargeted** screening: enabled environmental molecular differences according to the sampling locations



Acknowledgments

This poster fits within the NewSTHEPS project (BR/143/NEWSTHEPS) supported by BELSPO, www.newstheps.be

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