

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

S. Huysman<sup>1</sup>, F. Vanryckeghem<sup>2</sup>, L. Van Meulebroeck<sup>1</sup>, E. De Paep<sup>1</sup>, H. Van Langenhove<sup>2</sup>, K. Demeestere<sup>2</sup> and L. Vanhaecke<sup>1</sup>

<sup>1</sup> FACULTY OF VETERINARY MEDICINE, DEPARTMENT OF VETERINARY PUBLIC AND FOOD SAFETY, LABORATORY OF CHEMICAL ANALYSIS, MERELBEKE, BELGIUM

<sup>2</sup> FACULTY OF BIOSCIENCE ENGINEERING, DEPARTMENT OF SUSTAINABLE ORGANIC CHEMISTRY AND TECHNOLOGY, ENVIRONMENTAL ORGANIC CHEMISTRY AND TECHNOLOGY, GHENT, BELGIUM

## 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

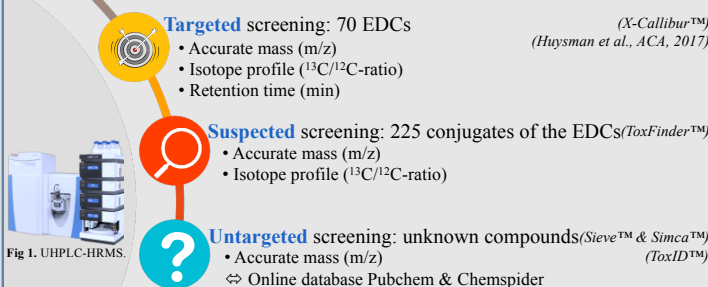
### Goals:

- 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

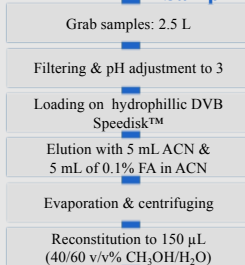


Fig 2. Optimised extraction protocol for grab samples obtained from the marine environment.

- Monitoring the Belgian Part of the North Sea (BPNS)
- 2 sampling campaigns, i.e. fall 2016 (1-4) & winter 2017 (5-7), at 4 different sampling locations:

- Harbour of Oostende: (1) & (5)
- Oostende Open Sea: (2) & (6)
- Harbour of Zeebrugge: (3) & (7)
- Zeebrugge Open Sea: (4)

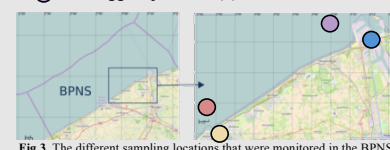
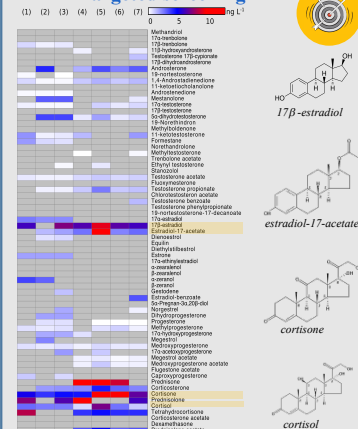


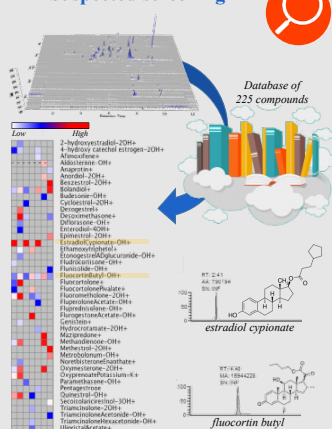
Fig 3. The different sampling locations that were monitored in the BPNS.

## Results

### Targeted screening



### Suspected screening



### Untargeted screening

#### Multi-variate analysis

- Scaling: pareto
- Transformation: log
- Compound Intensities > 10<sup>6</sup>

#### Legend

- (1) & (5): 51.2263°, 2.9357°
- (2) & (6): 51.2468°, 3.1136°
- (3) & (7): 51.3401°, 3.2003°
- (4): 51.3605°, 3.1136°
- Quality control

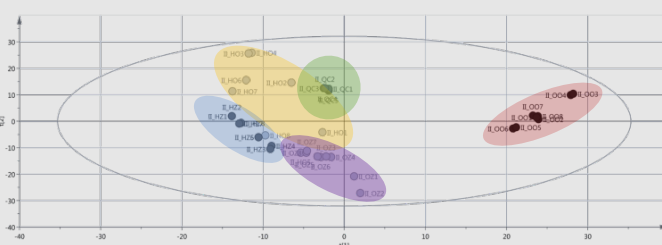


Fig 6. PCA-X Plot displaying the untargeted analysis of different sampling locations and periods in the positive ionization mode.

## 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 NewSTEPS project (BR/143/NEWSTEPS) supported by BELSPO, www.newstheps.be

### Contact

Steve.Huysman@Ugent.be  
 Lynn.Vanhaecke@Ugent.be  
 www.vvv.ugent.be

