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Introduction

A reliable identification of suspected organic micropollutants at trace levels in environmental samples requires integrated analytical workflows based on liquid chromatography coupled to high resolution mass spectrometry. The challenge for suspected screening strategy is to develop a systematic and generalizable workflow, based on the acquisition of general information on suspected compounds, with spectral and chromatographic data and on the confrontation of the acquired data to libraries or software tools. Such analytical strategy was already successfully applied to identify degradation products of selected micropollutants in waste waters during tertiary ozonation processes, in constructed wetlands downstream waste water treatment plants and also in surface waters from agricultural watersheds.

Materials and methods

A combined **targeted and suspected screening strategy** has been applied to various waters samples:

1 - Waste waters from treatment plants
 (pharmaceuticals, hormones, pesticides)



2 - Surface waters from agricultural watersheds
 (pesticides, veterinary drugs)

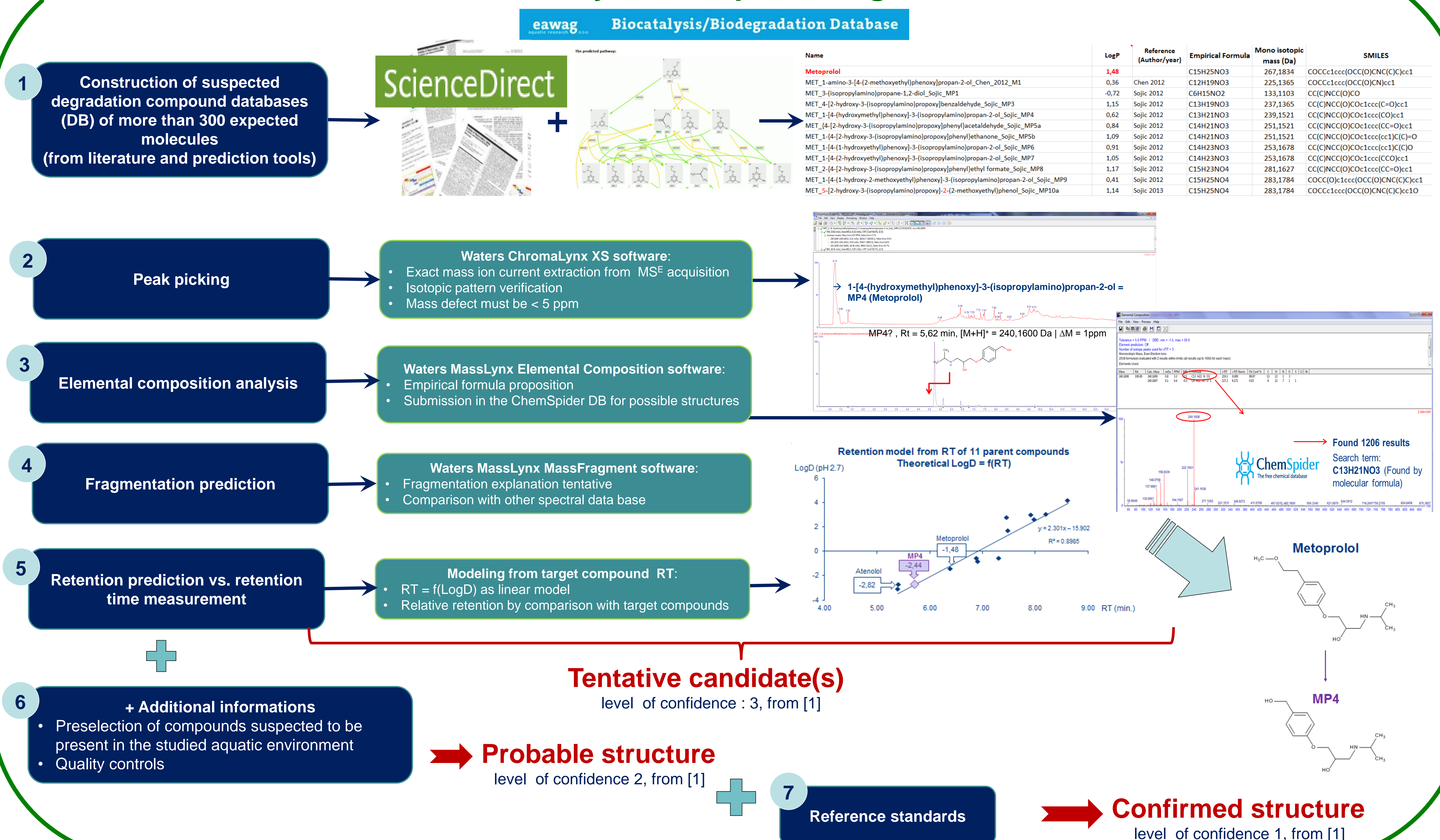


Analytical procedure

- Direct injection of filtered waters
- Analysis of parent and transformation products with a **Waters ACQUITY H-Class UPLC system coupled to a Xevo G2 S QTOF-HRMS**
- Separation on a C18 HSS-T3 column (100 x 2.1 mm, 1.8 µm - Waters)
- Data acquisition and processing with **TargetLynx** and **ChromaLynx** (MassLynx 4.1 software)
- **MS^E** acquisition mode (Data Independent Acquisition mode): low and high collision energy levels, sensitivity mode: resolution at 20000 (for 556,2771 Da)



General workflow – the case study of metoprolol degradation in constructed wetlands



Conclusions

- Development of a **successful analytical workflow** of screening strategy to identify degradation products in environmental case studies
- **Limitations:**
 - sample preparation: needs for sensitivity AND exhaustivity
 - data acquisition: differences between HRMS techniques and data formats → difficulty to share analytical databases
 - data treatment: time consuming → need for new software tools
 - data storage: problem of data size
 - confirmation **ONLY** with reference standards

References

[1] Schymanski E., et al. (2015). Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. *Analytical and Bioanalytical Chemistry*: 1-19.

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