Non-targeted screening of halogenated contaminants in a stranded killer whale (Orcinus orca) using GC-HRMS hyphenated with TIMS

Hugo Muller[1]; Krishna Das[2]; George Scholl[1]; Emma L. Schymanski[3]; Gauthier Eppe[1]

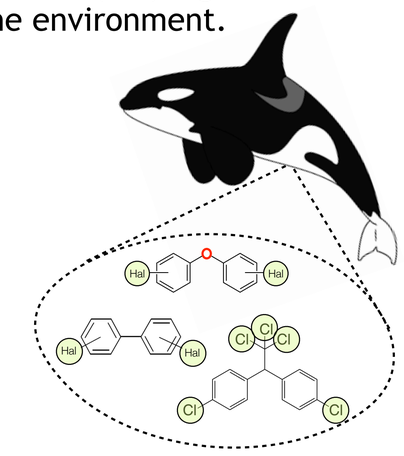
[1]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liège, Belgium
[2]Laboratory of Oceanology, Freshwater and Oceanic ScienCes Unit of ReSearch (FOCUS), University of Liège, Belgium
[3]Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg

Introduction

Persistent organic pollutants (POPs) are a class of chemical pollutants that were massively employed in agriculture and industry starting in the 1940's. Owing to their toxicity, resistance to (bio)degradation and bioaccumulation potential, they represent a significant threat for humans and the environment.

In 2004, the **Stockholm Convention** on POPs came into force with the aim to decrease and eliminate their use. However, restricted "**legacy**" POPs are still widespread in the environment. Moreover, many unrestricted "**emerging**" chemicals with POP-like properties have been discovered.

Killer whales are top-chain predators with a long lifetime. Therefore, they are at particularly high risk of being exposed to these POPs. Recent research indicates that killer whales are among the **most contaminated** animal species, which could account for their ongoing population decline worldwide.



Objective

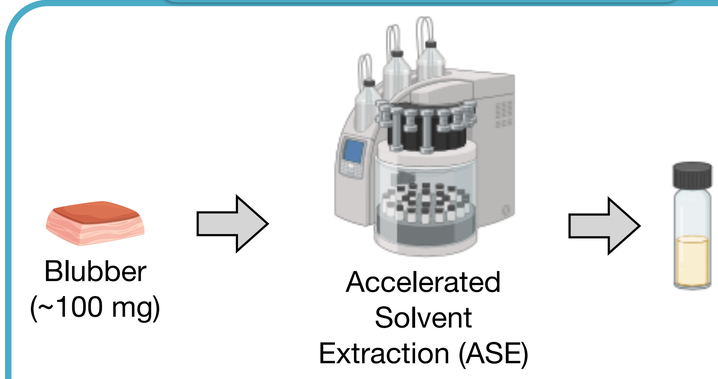
Beyond well-known **legacy** POPs, killer whale tissues likely contain various **emerging** and **unknown** contaminants, potentially leading to additional toxic impacts.

Identify **emerging POPs** in the blubber of a stranded killer whale, using an advanced separation and identification technique: GC-IM-MS

Sample preparation

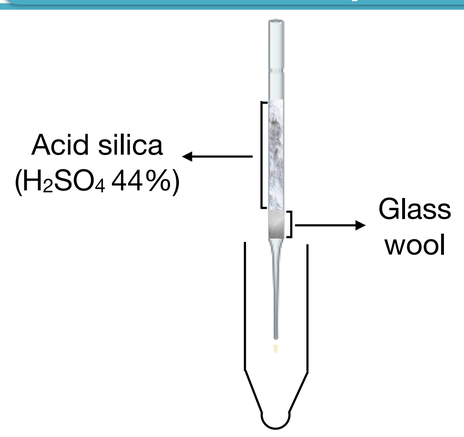
The sample preparation consisted of **two parts**

Extraction



Extraction of the fat, which contains the lipophilic POPs

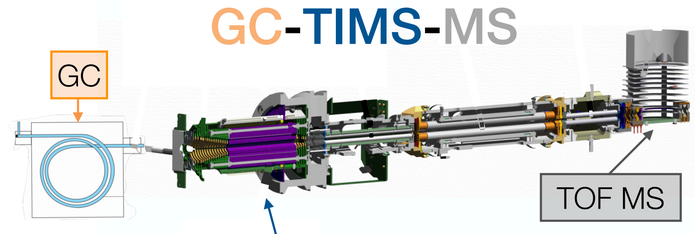
Clean-up

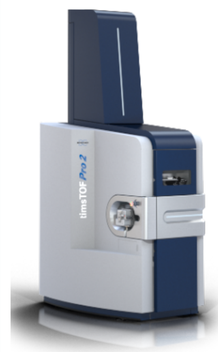


Clean-up to **eliminate** the fat

Instrumentation

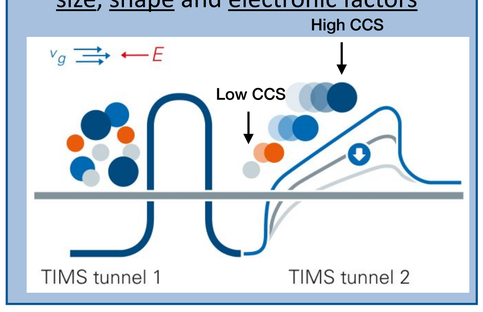
GC-TIMS-MS





Trapped ion mobility spectrometry

→ Ion separation according to size, shape and electronic factors



Non-targeted analysis

1 Prioritization: Ion mobility vs m/z heatmap

→ Halogenated compounds are **separated** from background and other non halogenated compounds in the heatmap

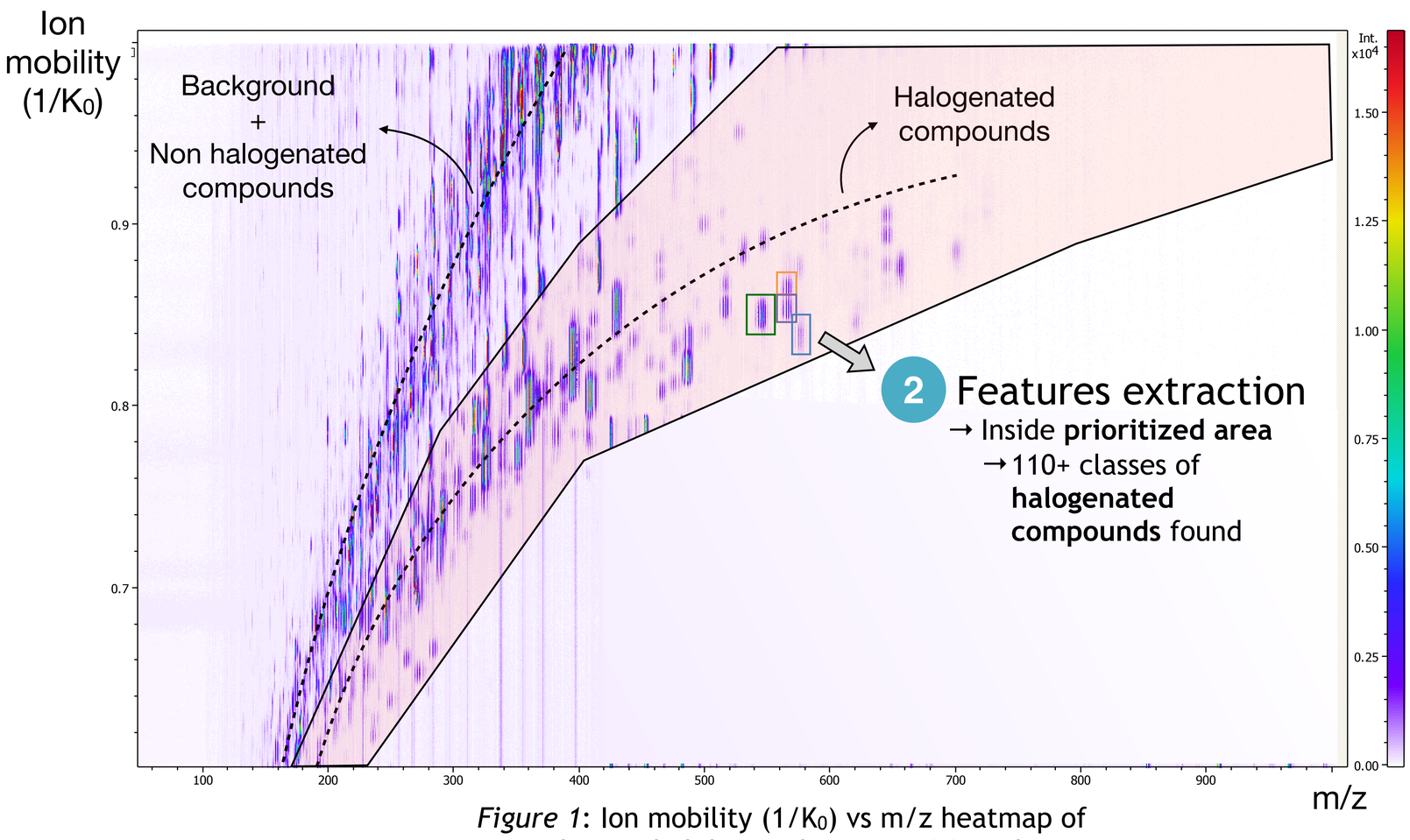
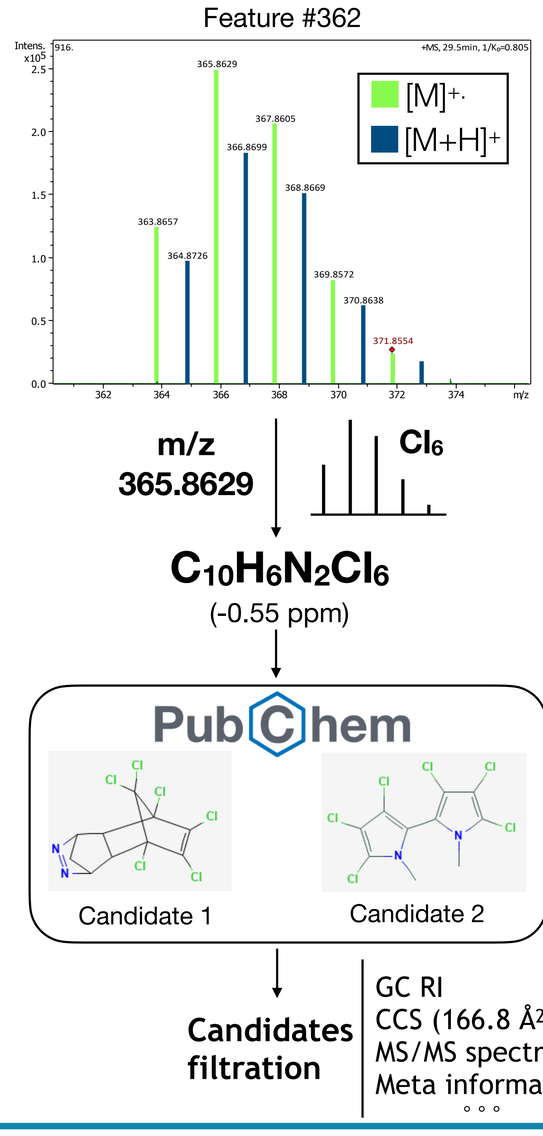


Figure 1: Ion mobility ($1/K_0$) vs m/z heatmap of signal recorded during the entire GC analysis

2 Features extraction

→ Inside **prioritized area**
→ 110+ classes of **halogenated compounds** found

3 Features identification



Conclusion

IM for NTA

The addition of **ion mobility** as a third dimension of separation improves **NTA** for halogenated compounds:
- **Increased selectivity**: background signal and non-halogenated ions are **separated** from analytes of interest
- **Feature identification**: **cleaner** mass spectra are obtained and use of **CCS** as an additional molecular descriptor

Killer whale contamination

Many different classes of potentially harmful halogenated compounds were found in the blubber of the killer whale. They will now require further **identification**.

H. Muller hugo.muller@uliege.be I **Prof. G. Eppe** g.eppe@uliege.be Mass Spectrometry Laboratory (MSLab) I www.mslab.uliege.be I MSLab_ULiege

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