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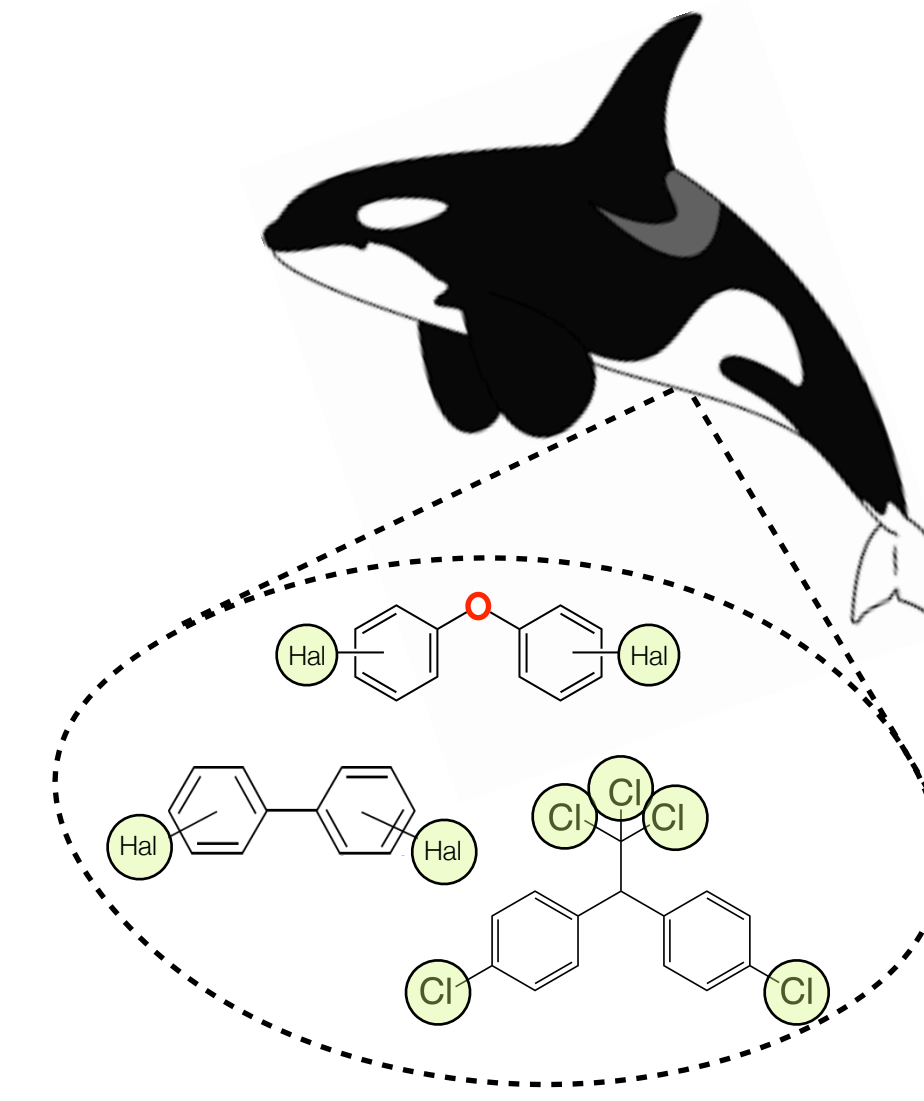
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Introduction

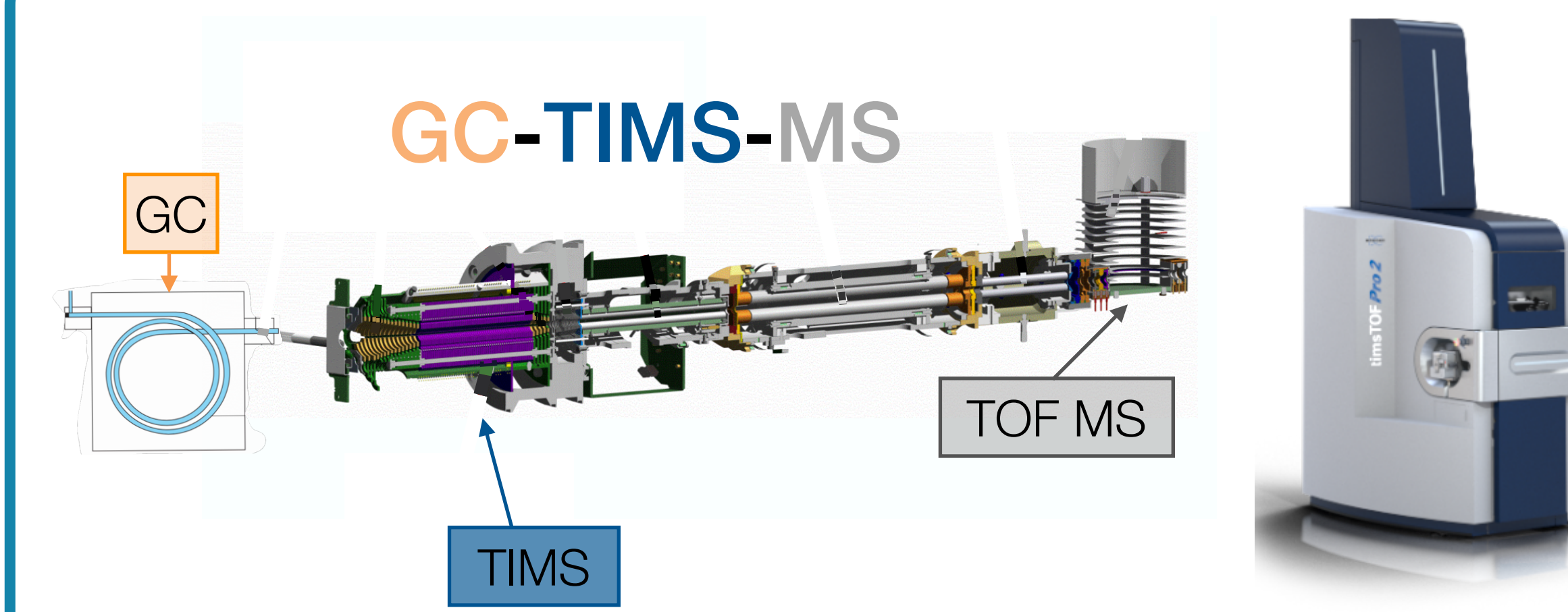
Persistent organic pollutants (POPs) are a class of chemical pollutants that were massively employed in agriculture and industry starting in the 1940's. Owing to their toxicity, resistance to (bio)degradation and bioaccumulation potential, they represent a significant threat for humans and the environment.

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.

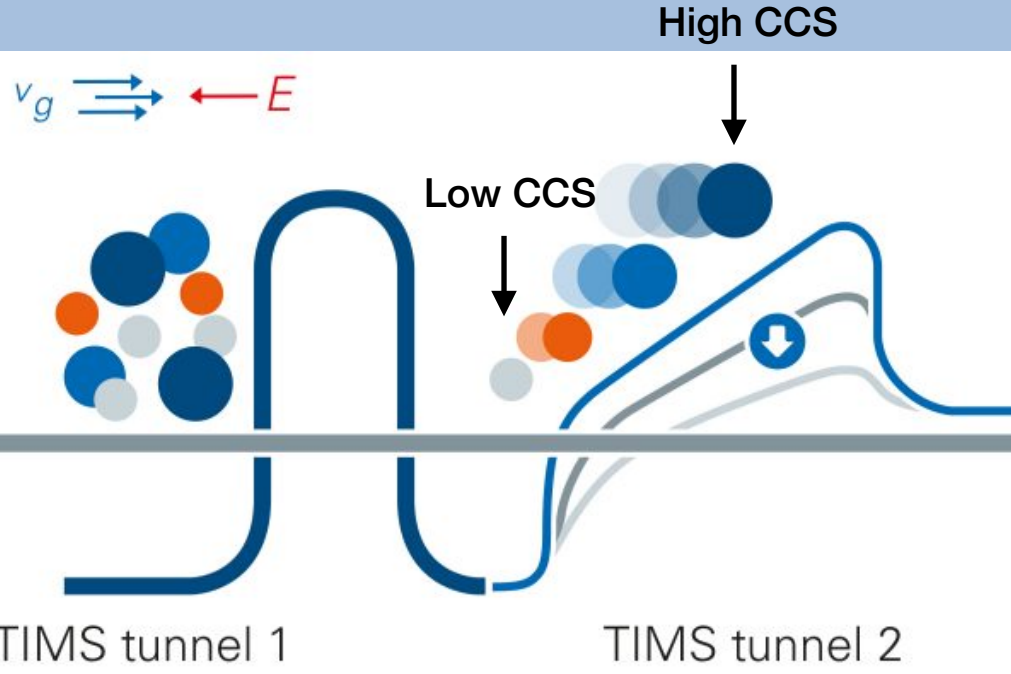


Instrumentation



Trapped ion mobility spectrometry

→ Ion separation according to size, shape and electronic factors



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.

Non-targeted analysis

Objective

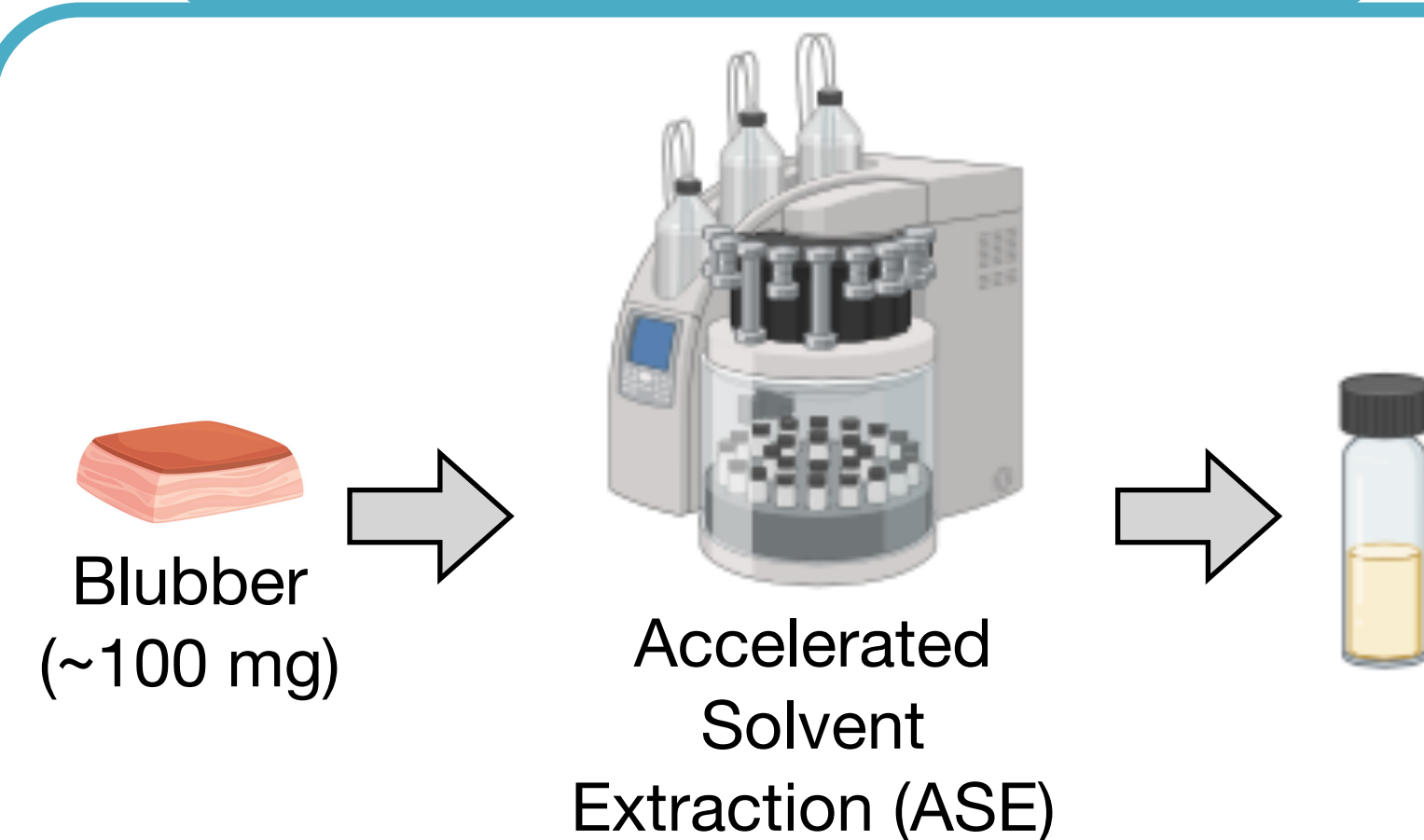
Beyond well-known **legacy** POPs, killer whale tissues likely contain various **emerging** and **unknown** contaminants, potentially leading to additional toxic impacts.

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

Sample preparation

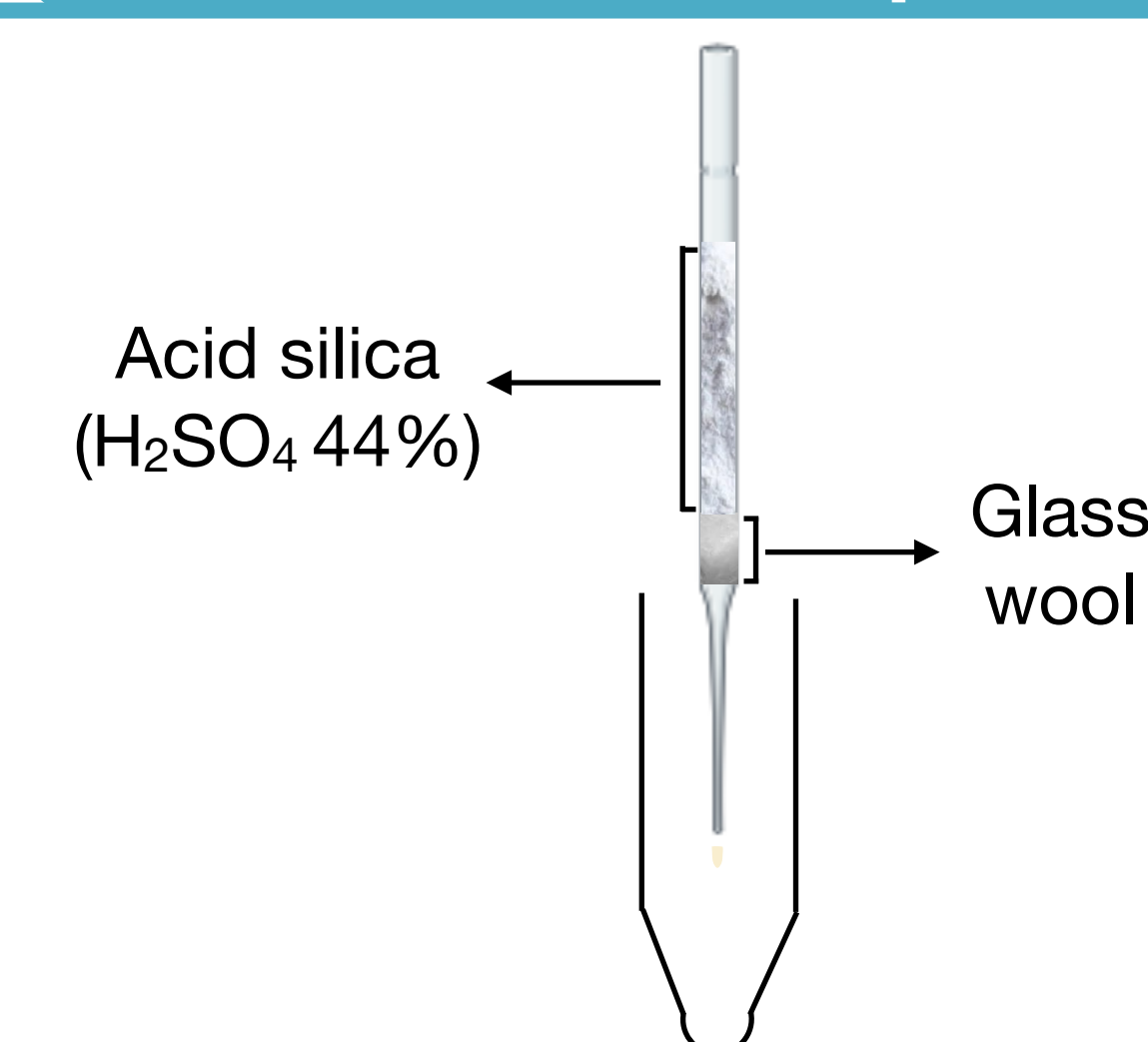
The sample preparation consisted of two parts

Extraction



Extraction of the fat, which contains the lipophilic POPs

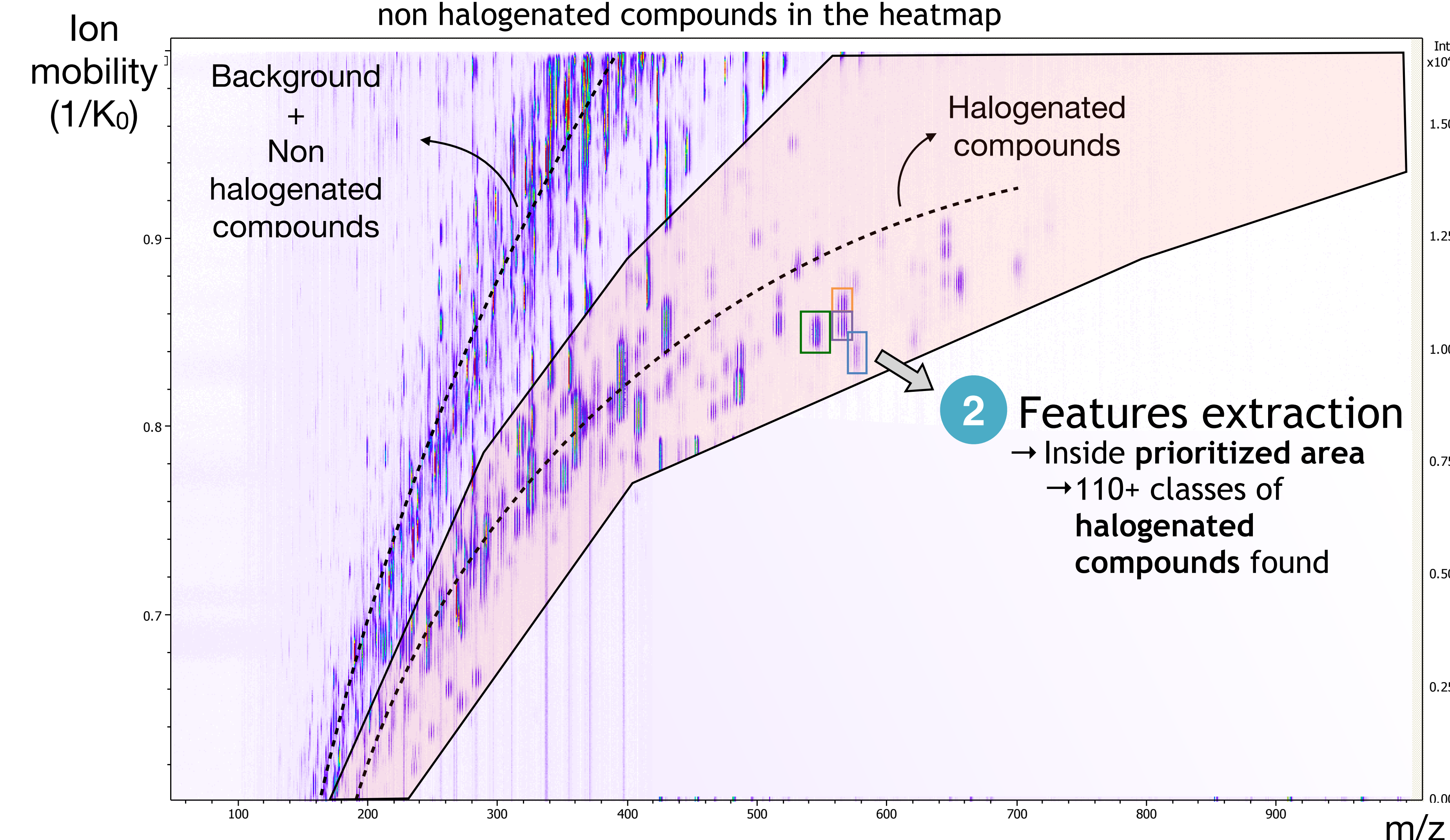
Clean-up



Clean-up to eliminate the fat

1 Prioritization: Ion mobility vs m/z heatmap

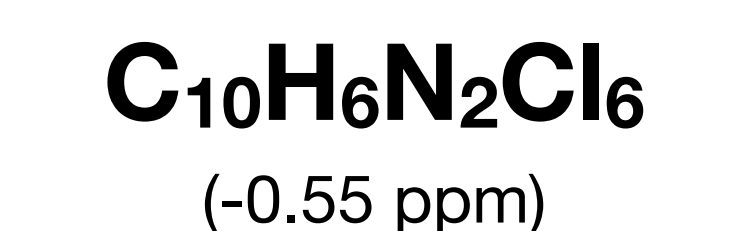
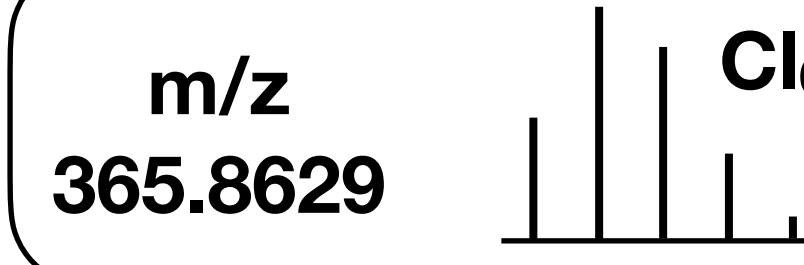
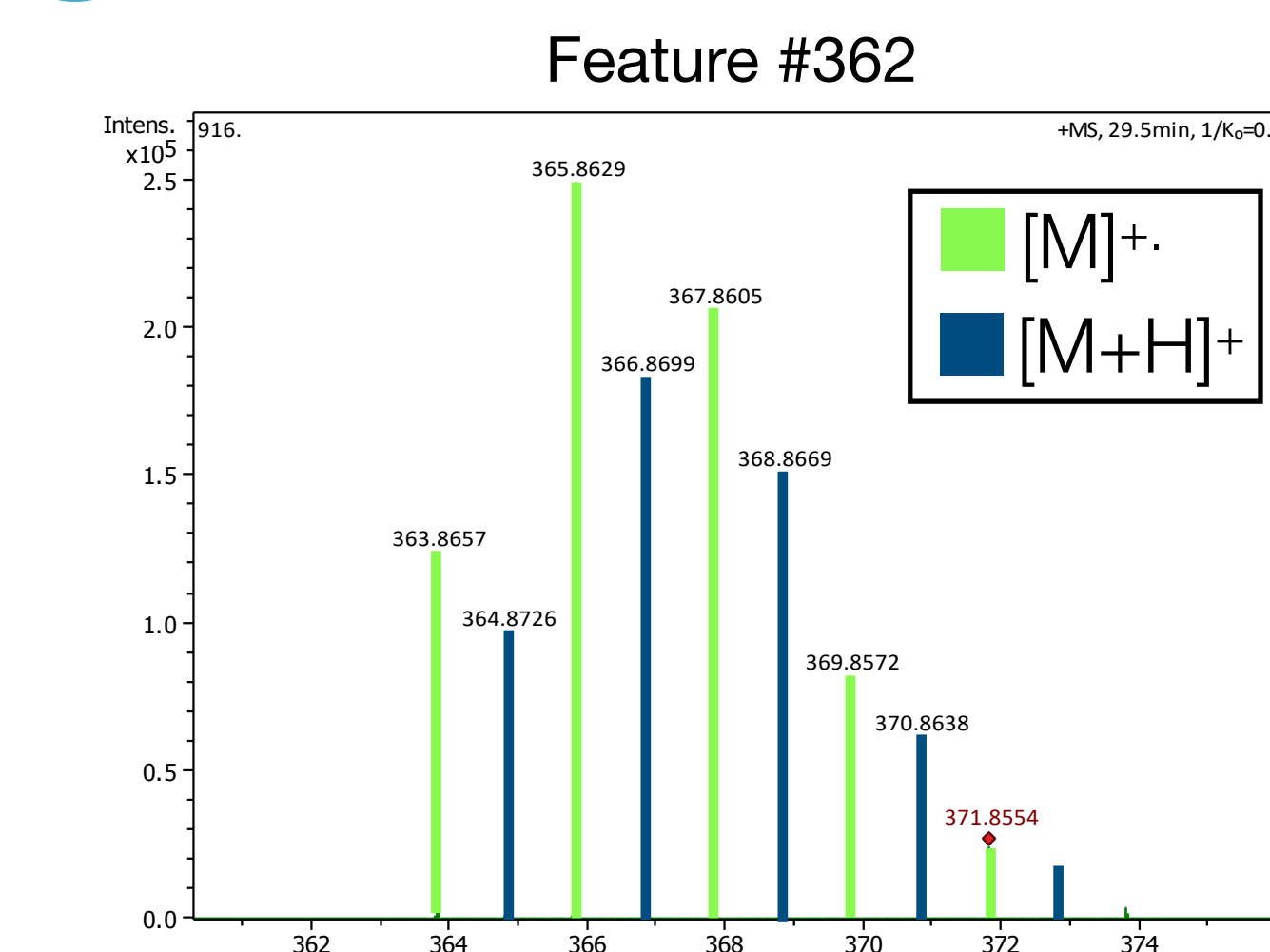
→ Halogenated compounds are separated from background and other non halogenated compounds in the heatmap



2 Features extraction

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

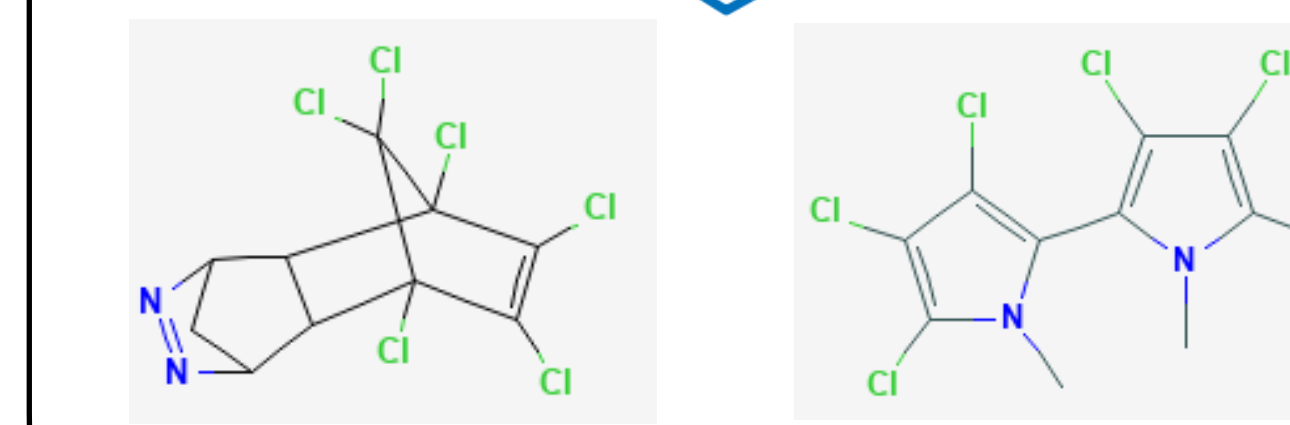
3 Features identification



Candidates filtration

GC RI
CCS (166.8 Å²)
MS/MS spectra
Meta information

PubChem



Candidate 1 Candidate 2

Figure 1: Ion mobility (1/K₀) vs m/z heatmap of signal recorded during the entire GC analysis