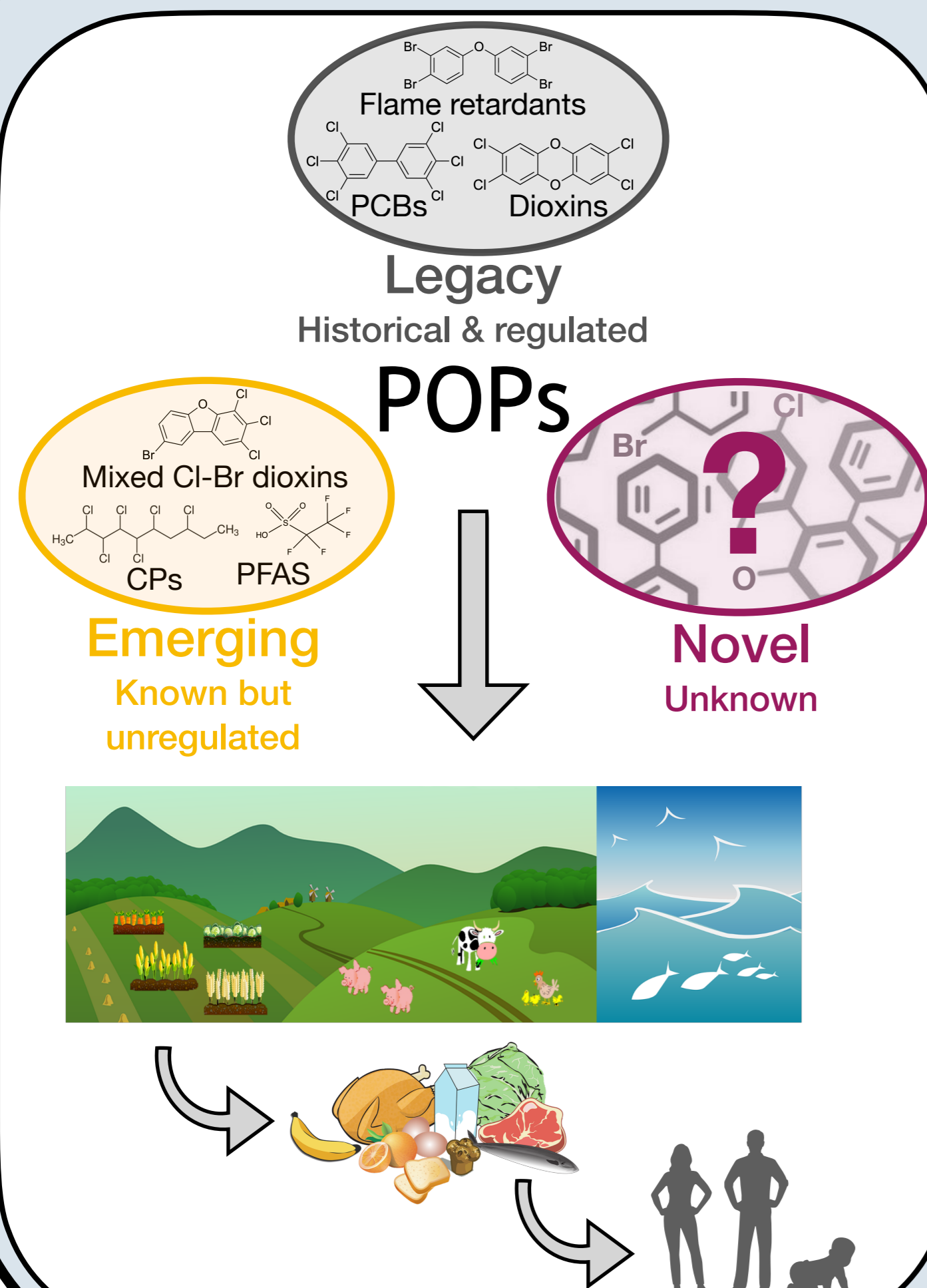


INTRODUCTION

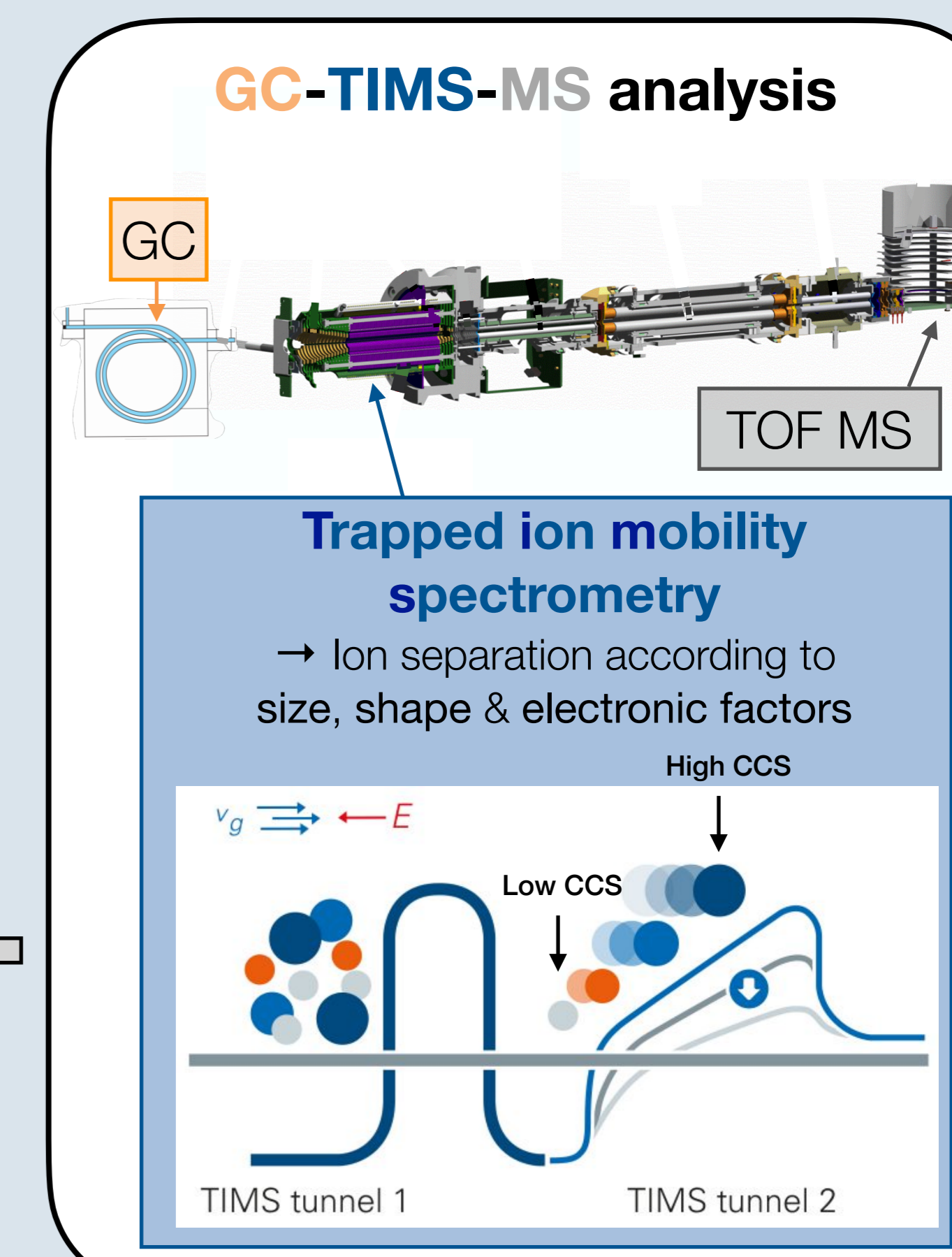
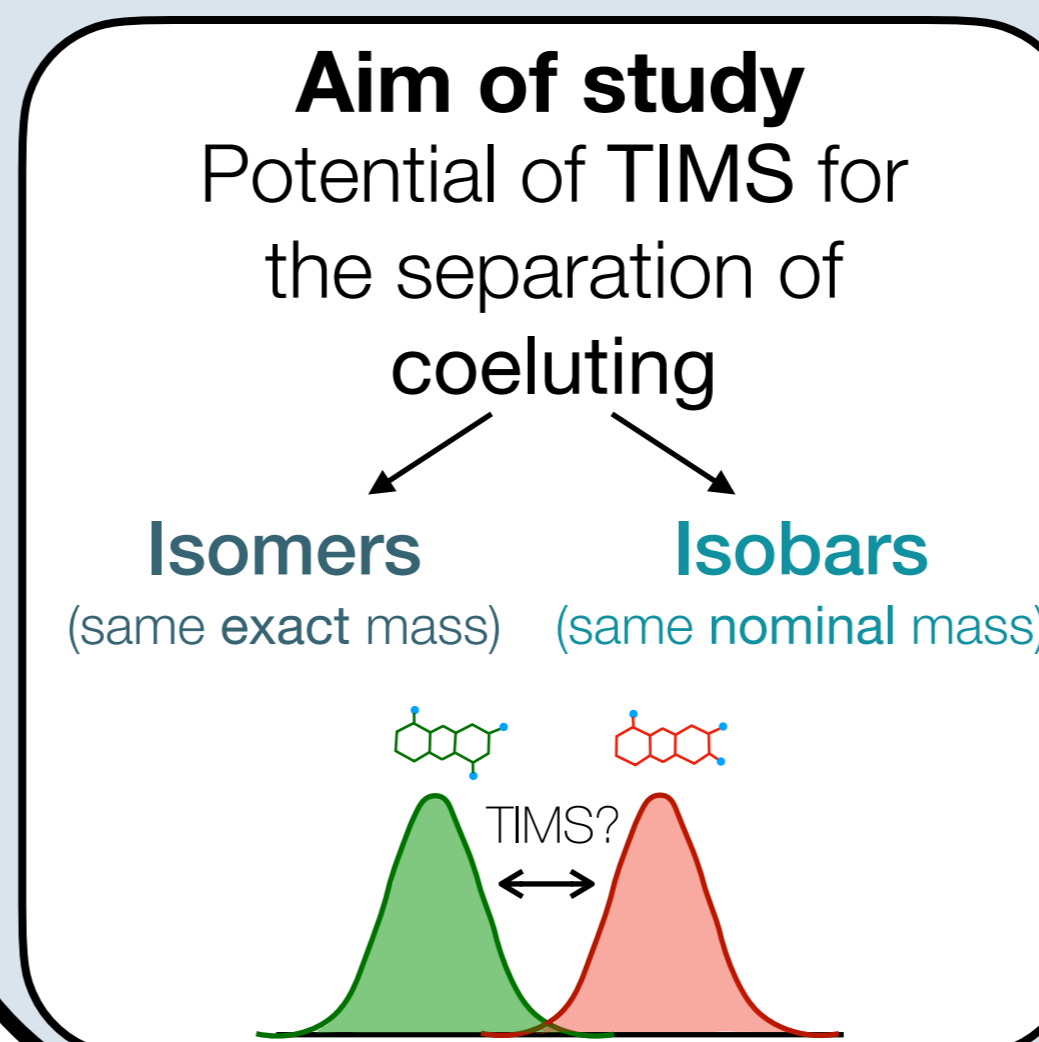
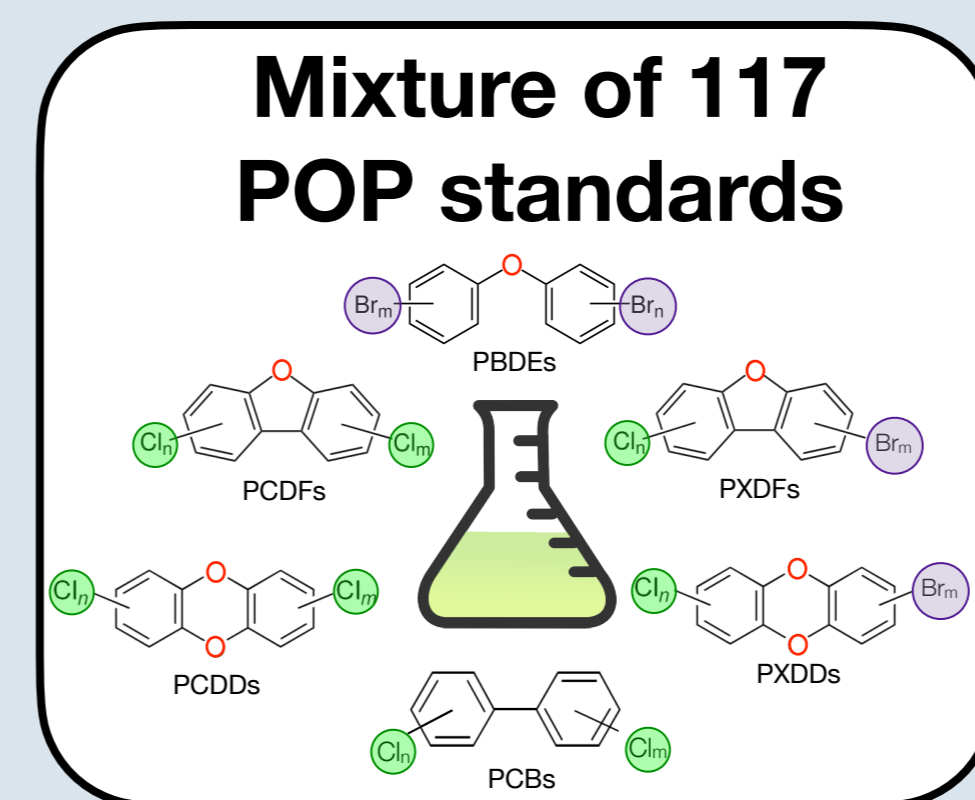


Nowadays, the ubiquitous presence and continuous emission of a wide range of pollutants in the environment is of particular concern due to the adverse effects they represent for human kind and ecosystems.

In particular, the monitoring of halogenated persistent organic pollutants (POPs) is based mostly on targeted GC-MS approaches. However, with the increasing number of contaminants to be monitored, novel analytical methods that allow rapid screening and quantitation of multiple POPs simultaneously are in high demand.

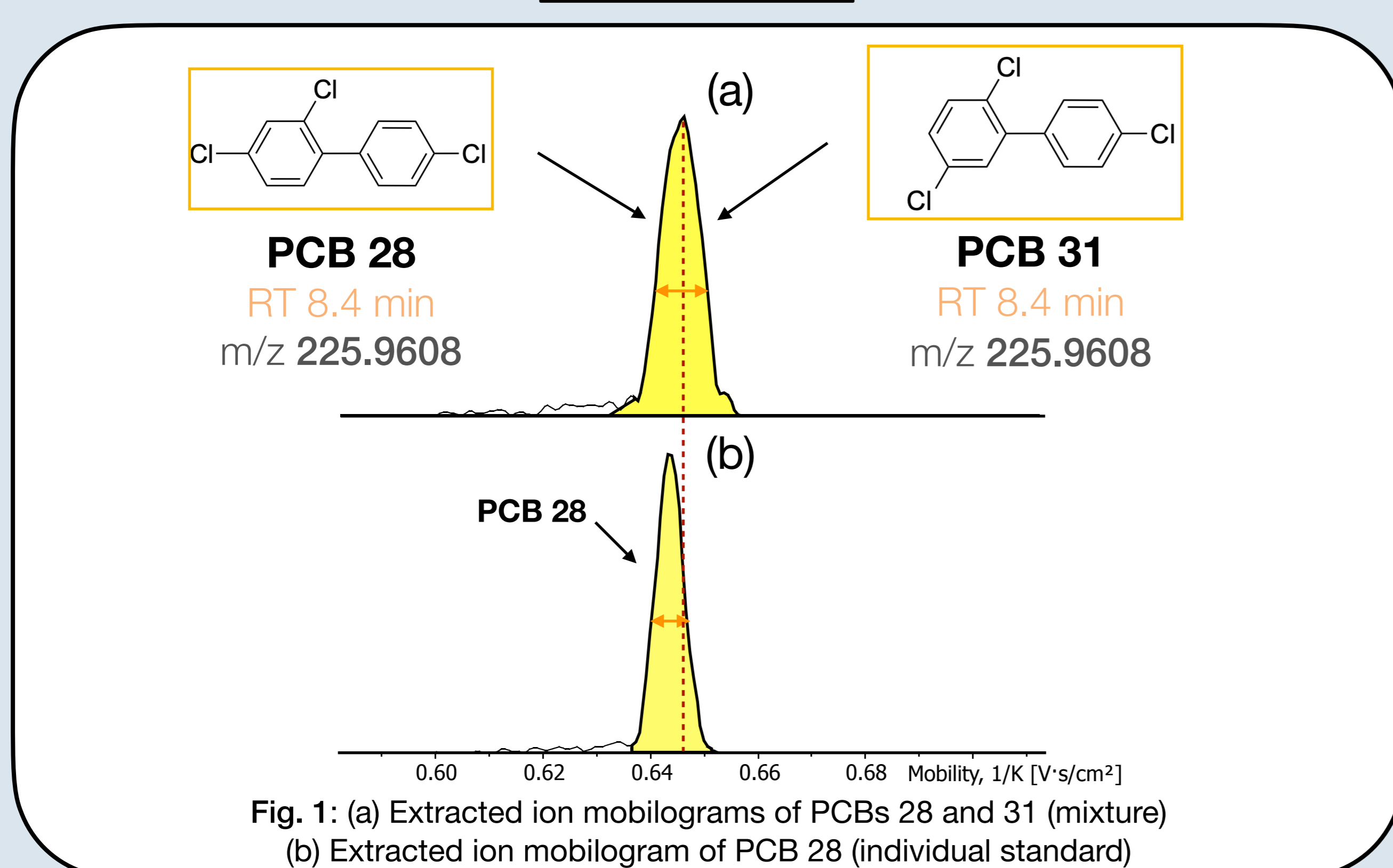
In this context, we propose to develop a novel quantitative, non-targeted analytical strategy that relies on the hyphenation of trapped ion mobility spectrometry (TIMS) with GC-MS to probe and monitor halogenated POPs in complex food/environmental samples.

MATERIAL & METHODS



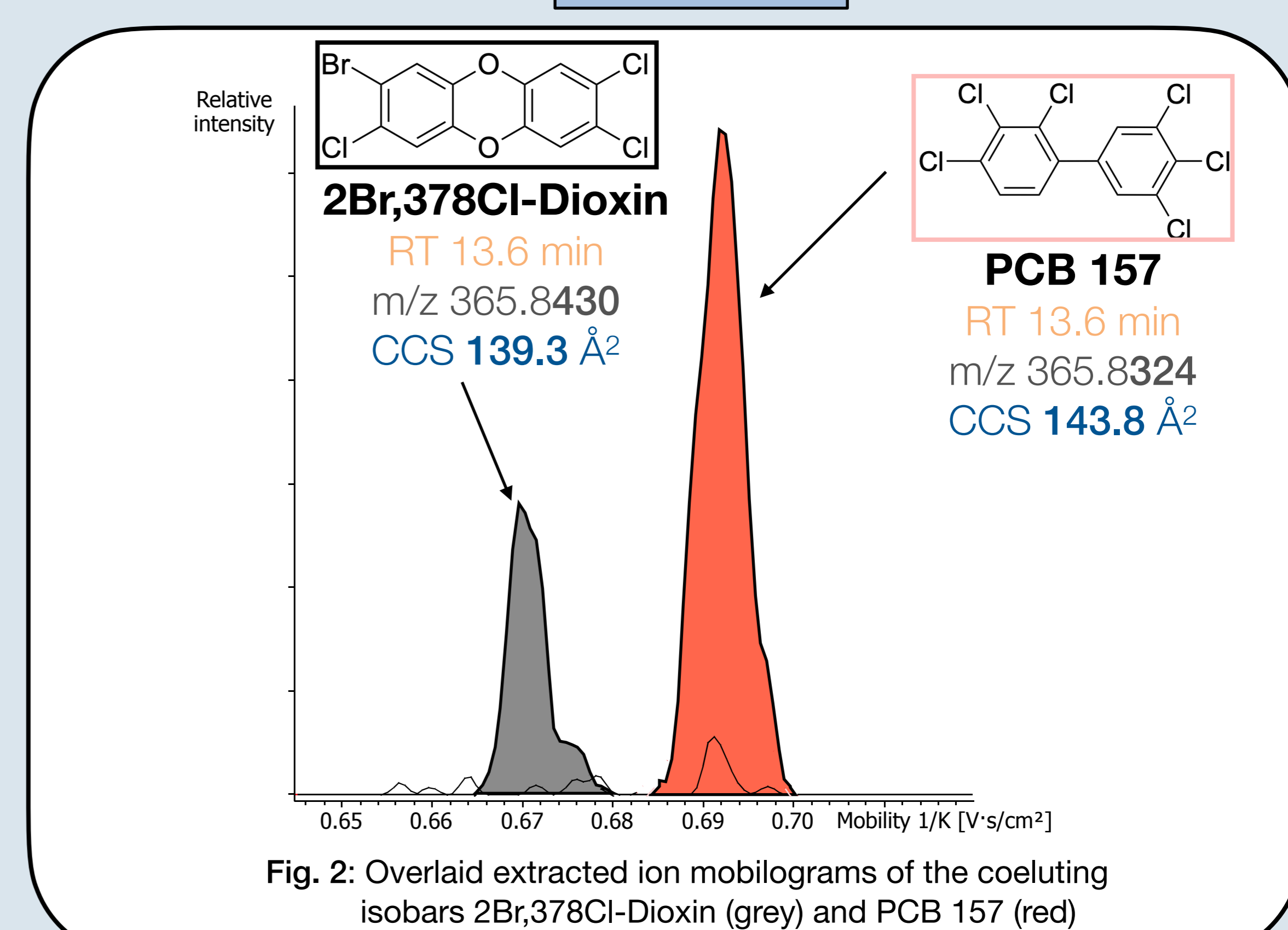
RESULTS & DISCUSSION

Isomers



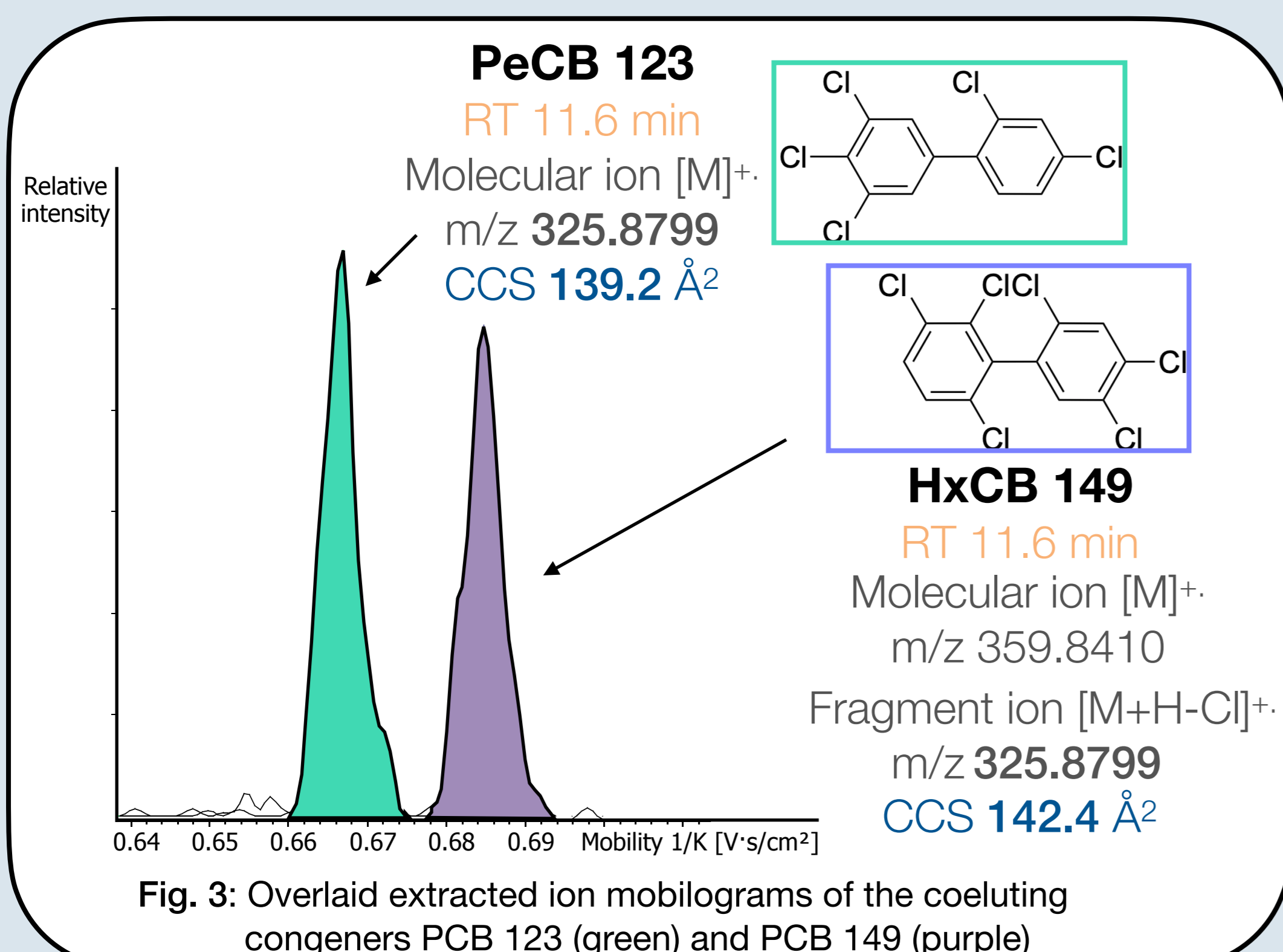
- Coeluting isomeric congeners usually have very close CCS values
- Comparison with ion mobility peak of PCB 28 alone (FWHM & peak maximum) suggests that the two TriCBs have slightly different CCS values. This is consistent with one literature value¹ which measured $\Delta\text{CCS} = 0.7\%$ for these PCBs
- Even with the high ion mobility resolving power achieved in TIMS ($R \sim 116$), only partial separation of coeluting isomeric congeners can be achieved

Isobars



- Coeluting isobaric pollutants with nearly identical mass are readily separated by TIMS, owing to their difference in CCS
- In the example given, 2Br,378Cl-Dioxin and PCB 157 are base line resolved in the ion mobility dimension ($\Delta\text{CCS} = 3.2\%$)

Isomeric fragments



- In a typical APCI-TIMS-MS experiment, fragmentation of molecular ions can occur if they acquire sufficient internal energy (e.g., in source, during transfer, trapping, ...)
- Coelution of halogenated POP congeners which differ by one degree of halogenation is common. While the molecular ions M^+ are readily differentiated in the m/z dimension (e.g., m/z 325 and 359 for PCBs 123 & 149 respectively), formation of $[M+H-X]^+$ fragment ions (where X is a halogen atom) from the congener with the highest halogenation degree (PCB 149) can lead to severe isomeric interference with the molecular ion of the congener with the lowest halogenation degree (PCB 123)
- With TIMS, isomeric $[M+H-X]^+$ fragment ions formed:
 - Before or during TIMS separation are difficult to separate from the molecular ion of the congener with the lowest halogenation degree because both have similar ion mobility
 ➤ **Interference**
 - After TIMS separation do not interfere because the molecular ion of the congener with the lowest halogenation degree is base line separated in the ion mobility dimension from the parent ion of the fragment
 ➤ **No interference**

CONCLUSION

TIMS provides enhanced selectivity compared to more traditional GC-MS approaches. The added ion mobility dimension of separation enables the full discrimination of coeluting isobars and, to some extent, of coeluting isomers and isomeric fragments, demonstrating the potential of TIMS for the non-targeted analysis of complex halogenated contaminant mixtures.

Acknowledgement

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FREEDOM TO RESEARCH