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## **HaloSeeker, a user-friendly software to highlight halogenated chemicals in non-targeted HRMS data sets: presentation and overview of applications**

Ronan Cariou, Sébastien Hutinet, Yann Guitton, Mathilde Godere, Bruno Le Bizec, Jean-Philippe Antignac, Gaud Dervilly

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# HaloSeeker, a user-friendly software to highlight halogenated chemicals in non-targeted HRMS data sets: presentation and overview of applications

Ronan CARIOU, Sébastien HUTINET, Yann GUITTON, Mathilde GODÉRE, Bruno LE BIZEC, Jean-Philippe ANTIGNAC, Gaud DERVILLY



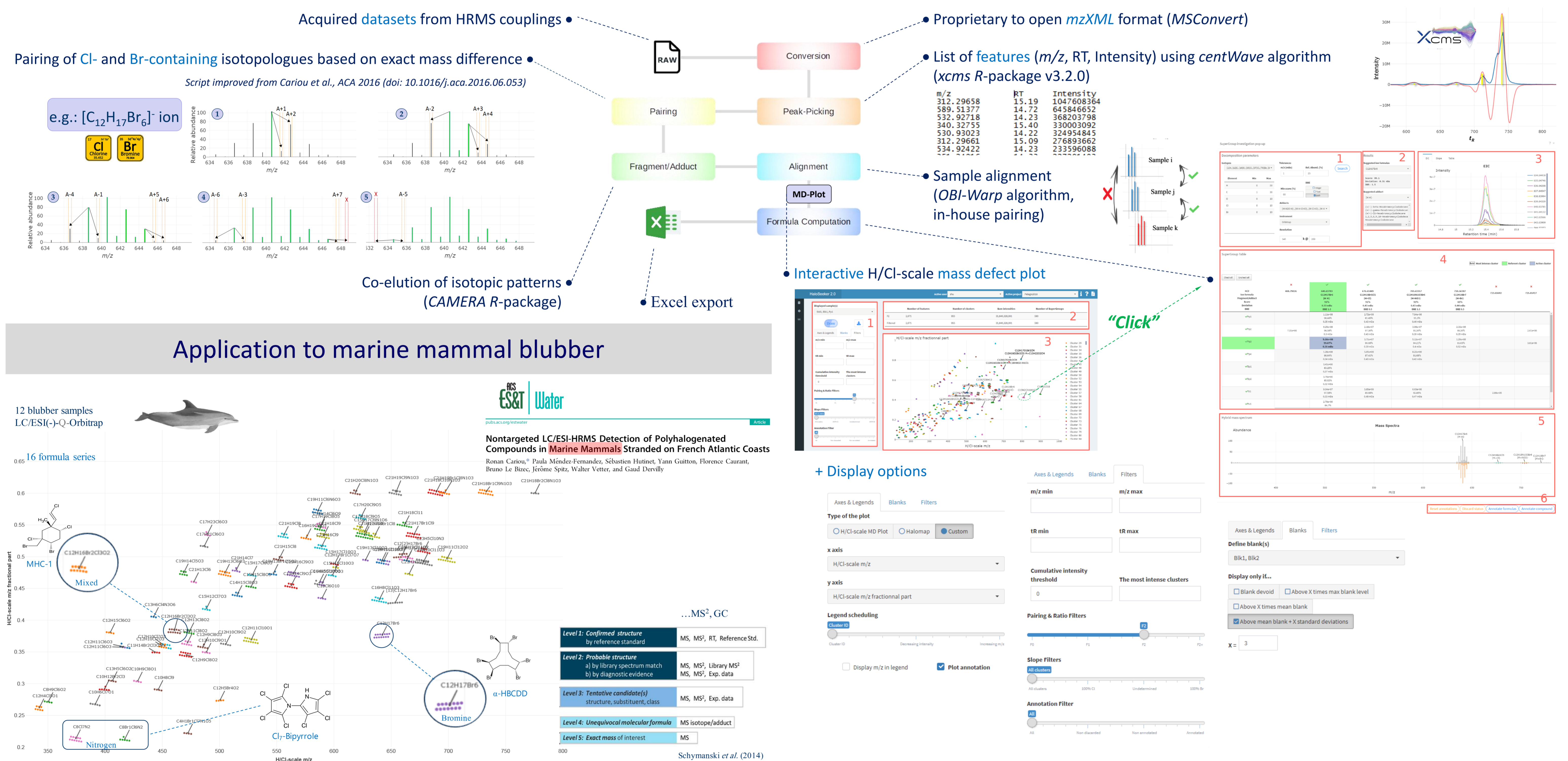
Oniris, INRAE, LABERCA, Nantes, France  
 Fax : +33 (0)2 40 68 78 78 - Tél : +33 (0)2 40 68 78 80  
 laberca@oniris-nantes.fr



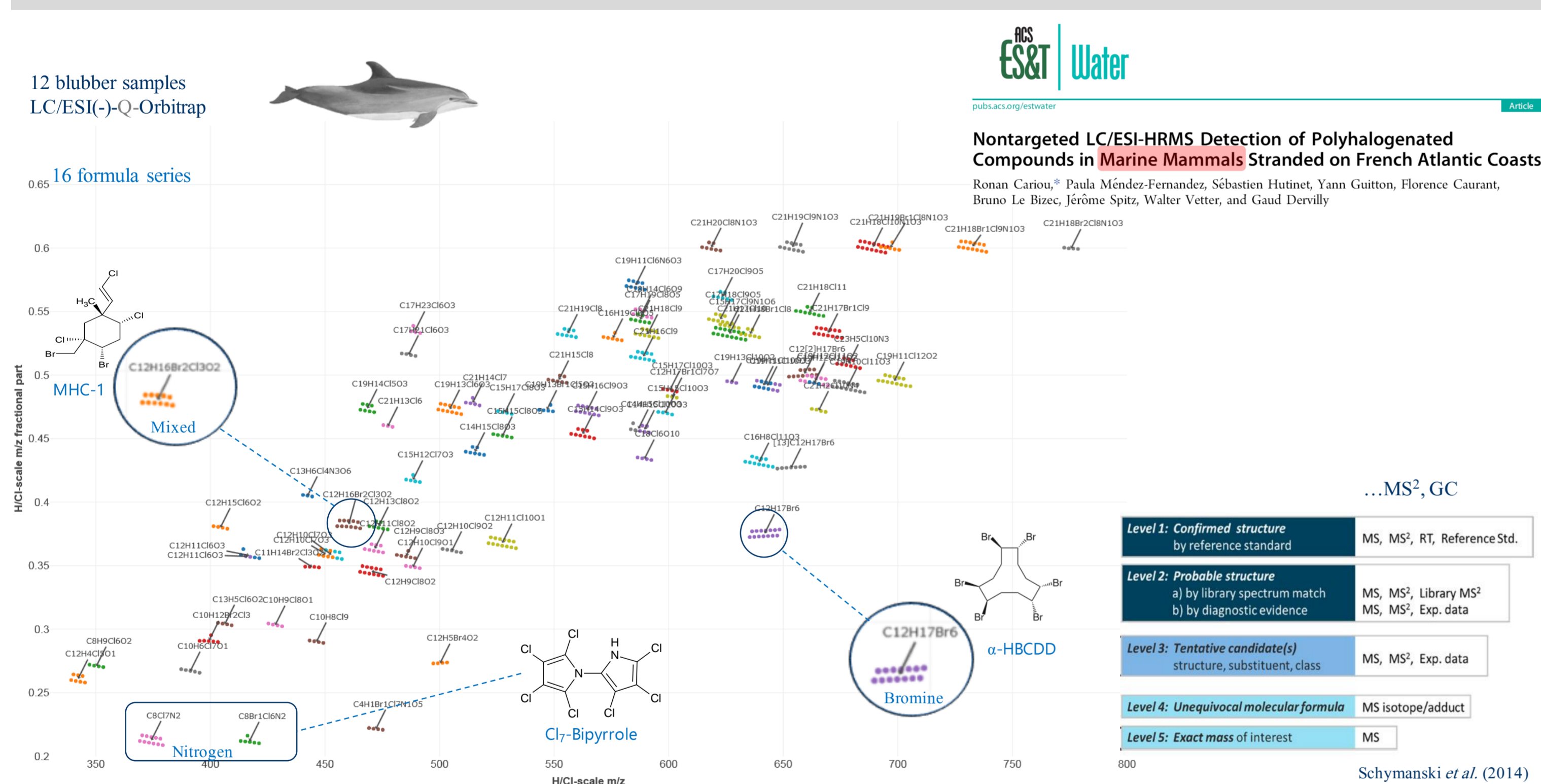
## Introduction

HaloSeeker is an **open-source software** aiming to seek **halogenated signatures** in full scan one-dimensional **HRMS fingerprints**. It is freely available on request at [contact.haloseeker@oniris-nantes.fr](mailto:contact.haloseeker@oniris-nantes.fr), under the GPLv3 license. The ergonomic **web user interface** in the *R* programming environment avoids any interactions with the coding component while allowing interactions with the data.

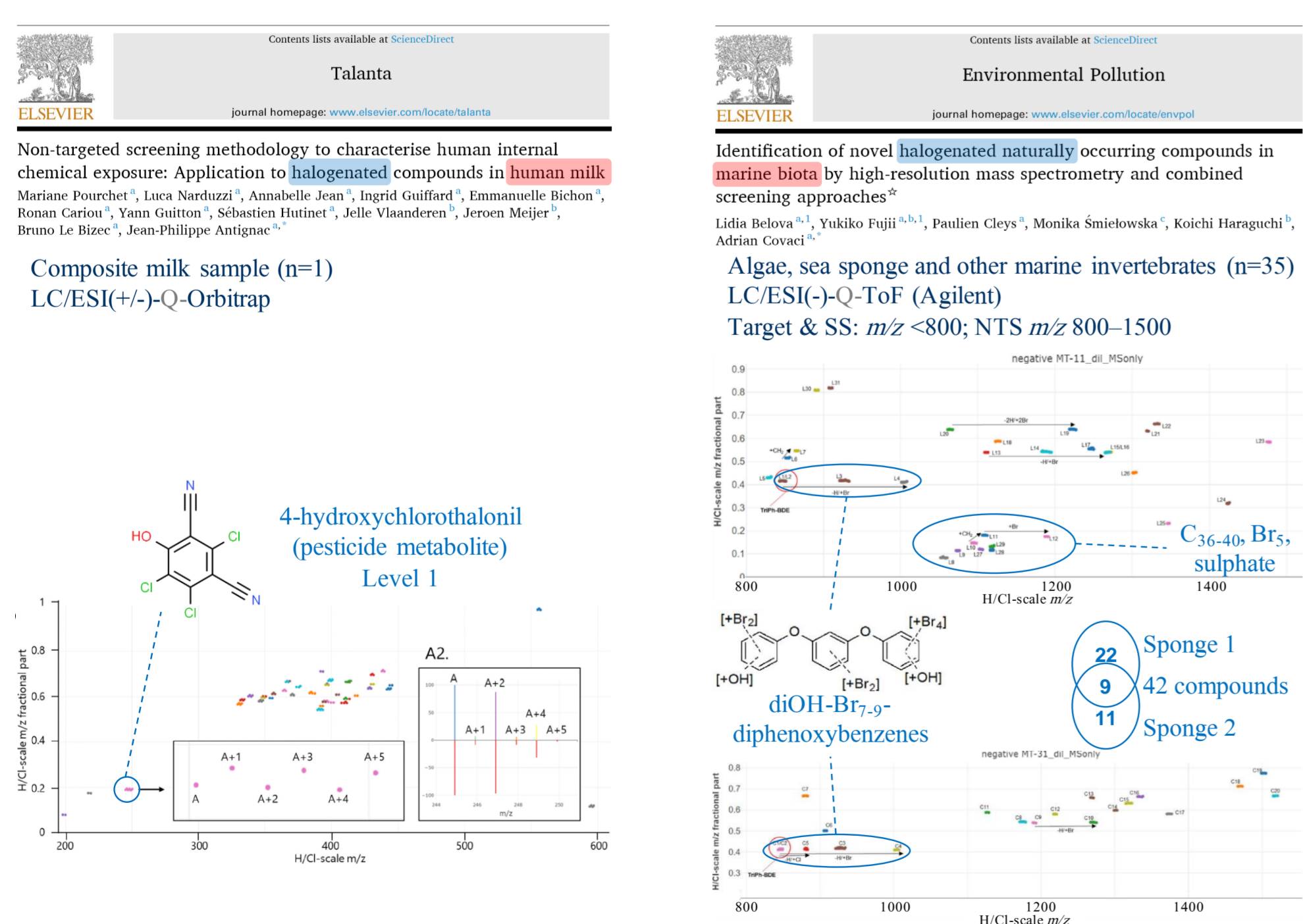
## Workflow



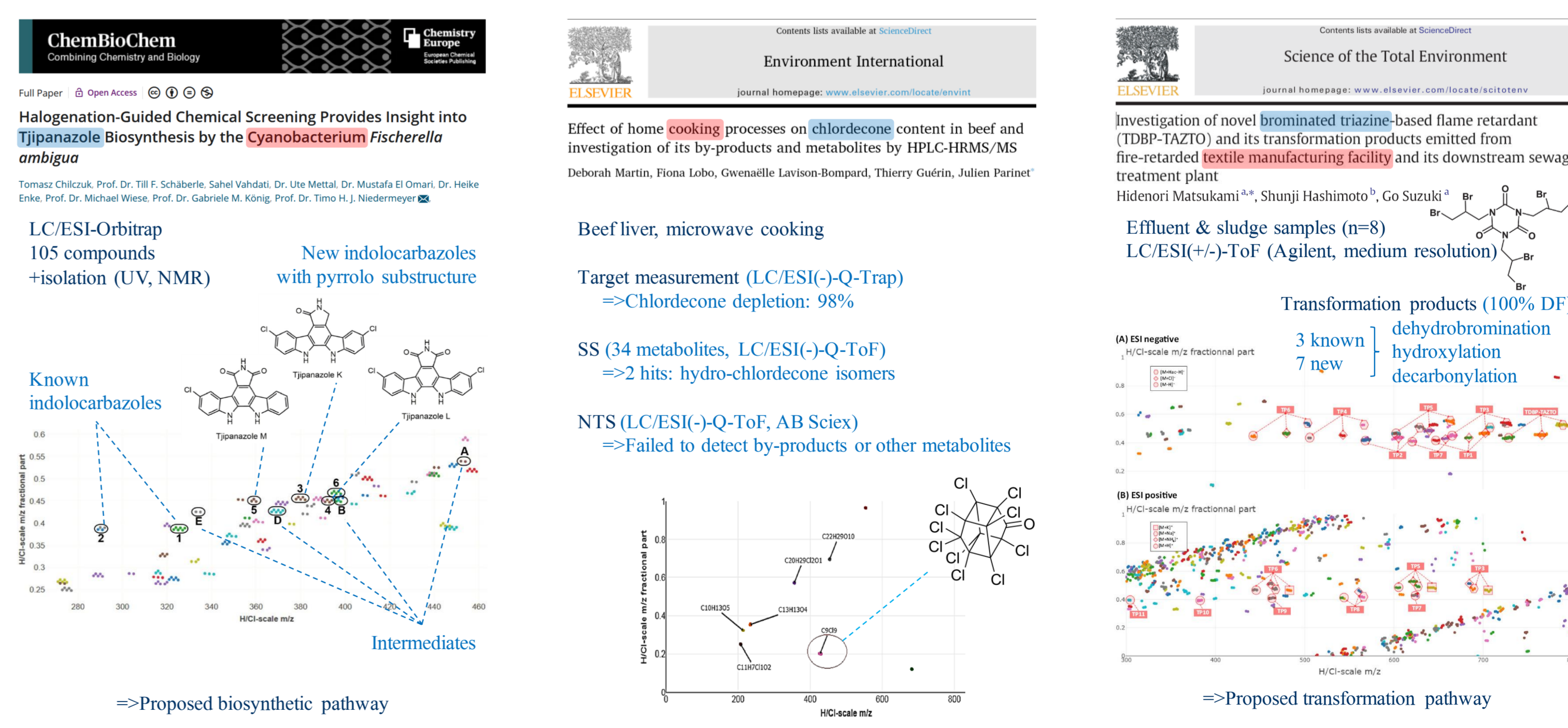
## Application to marine mammal blubber



## Applications to NTS



## Applications to biotransformation products



## Conclusion

Version 1.0, described by Léon *et al.* in 2019 (DOI: 10.1021/acs.analchem.8b05103), has been tested by 53 teams worldwide (22 countries). Citations of the work published in 2019 illustrate the diversity of applications, either in non-targeted studies or for (bio)transformation products identification. Users feedback allowed to release a version 2.0 in early 2021, offering numerous ergonomic improvements and script optimizations for a faster processing. So far, 51 teams worldwide downloaded this upgraded version.