



HAL
open science

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

► To cite this version:

Ronan Cariou, Sébastien Hutinet, Yann Guitton, Mathilde Godere, Bruno Le Bizec, et al.. HaloSeeker, a user-friendly software to highlight halogenated chemicals in non-targeted HRMS data sets: presentation and overview of applications. 10th International Symposium on Flame Retardants, Sep 2022, Athenes, Greece. 2022. hal-04264446

HAL Id: hal-04264446

<https://hal.science/hal-04264446v1>

Submitted on 30 Oct 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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



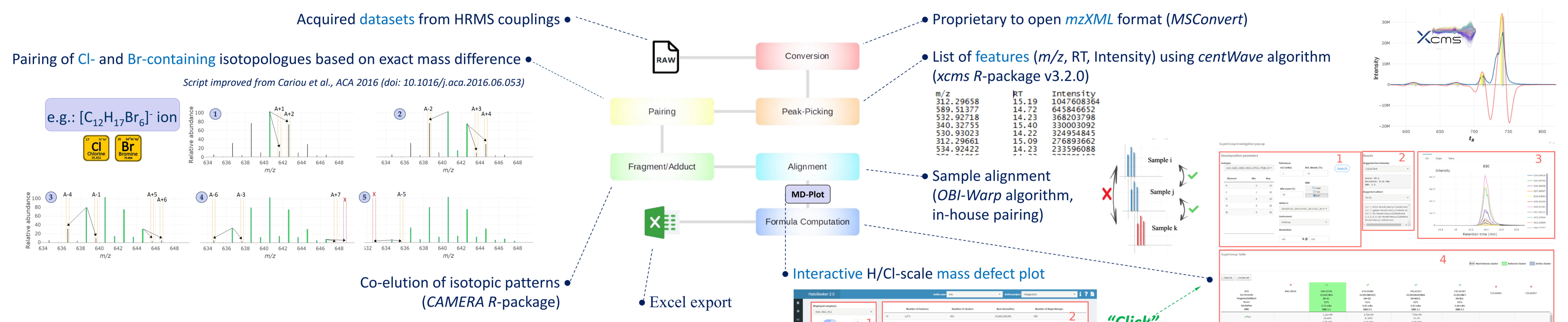
Oniris, INRAE, LABERCA, Nantes, France
 Fax : +33 (0)2 40 68 78 78 - Tél : +33 (0)2 40 68 78 80
 laberca@oniris-nantes.fr



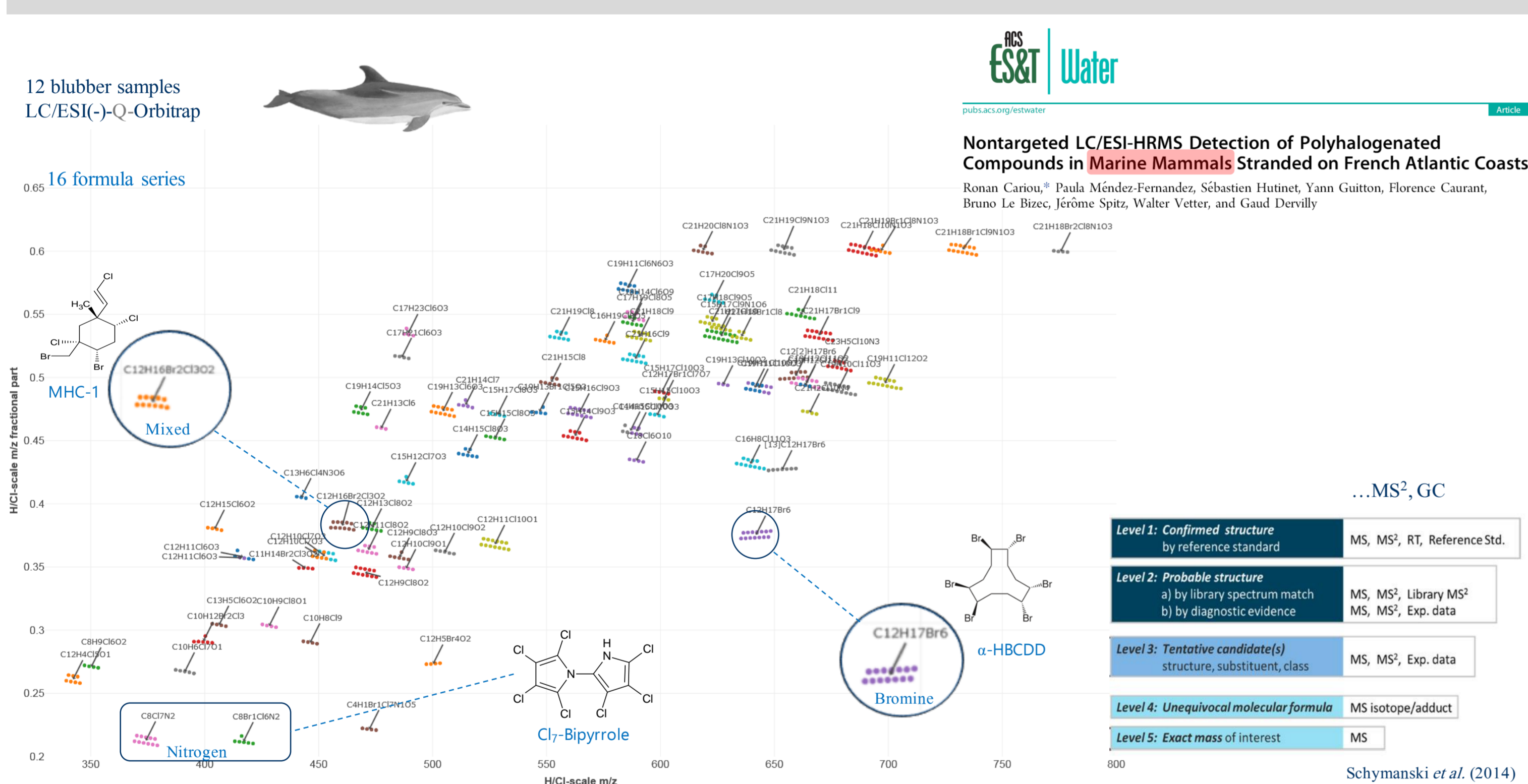
Introduction

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, 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.

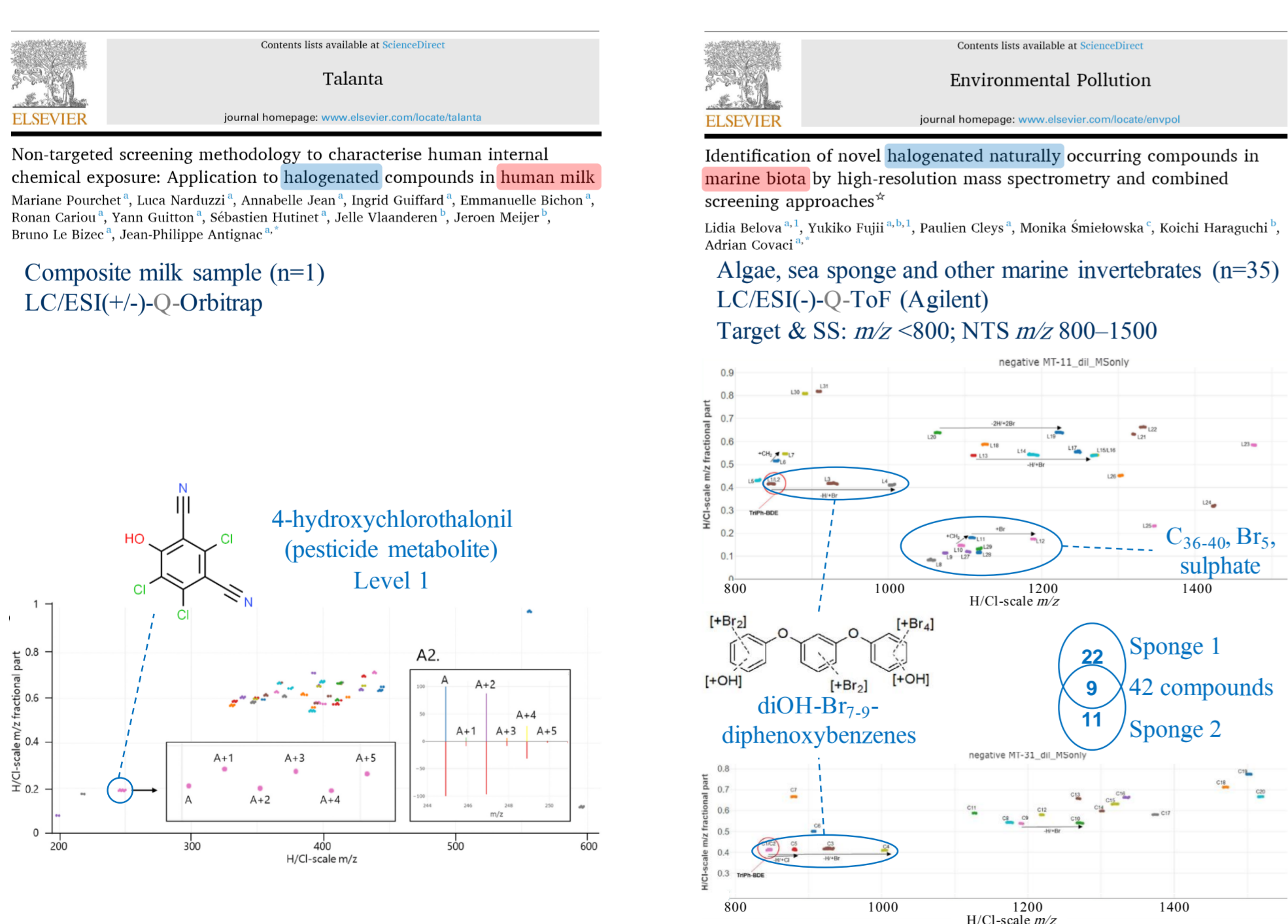
Workflow



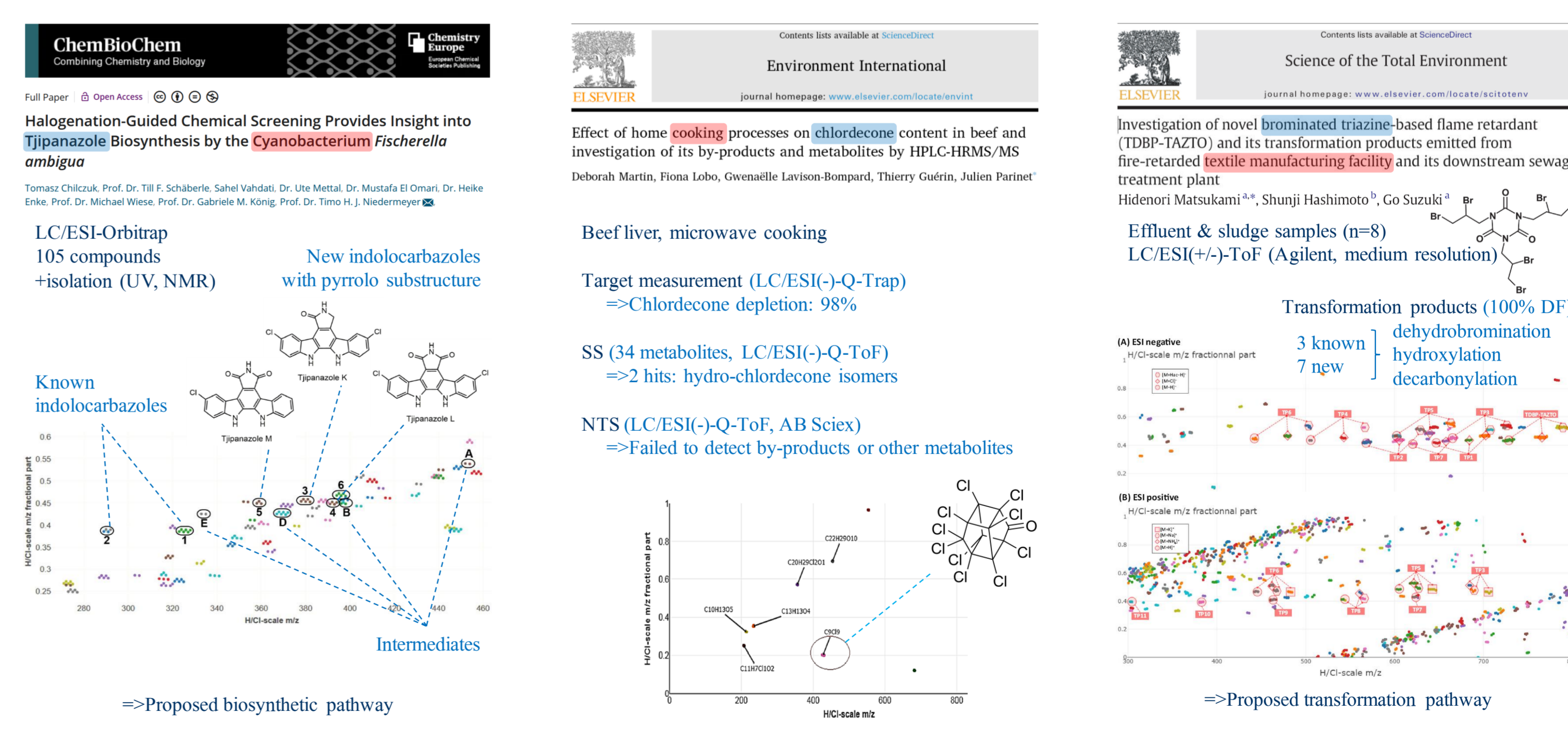
Application to marine mammal blubber



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.