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

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► To cite this version:

Ronan Cariou, Sébastien Hutinet, Yann Guitton, Tarek Moufawad, 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. *Analytics* 2022, Sep 2022, Nantes, France. 2022. hal-04264433

HAL Id: hal-04264433

<https://hal.science/hal-04264433>

Submitted on 30 Oct 2023

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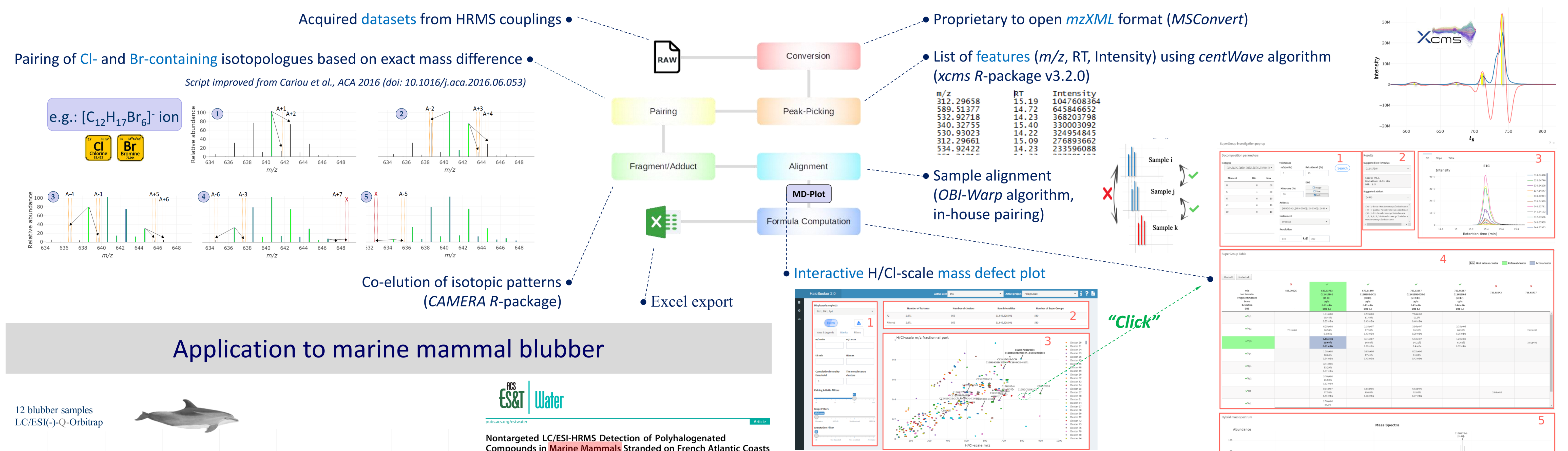
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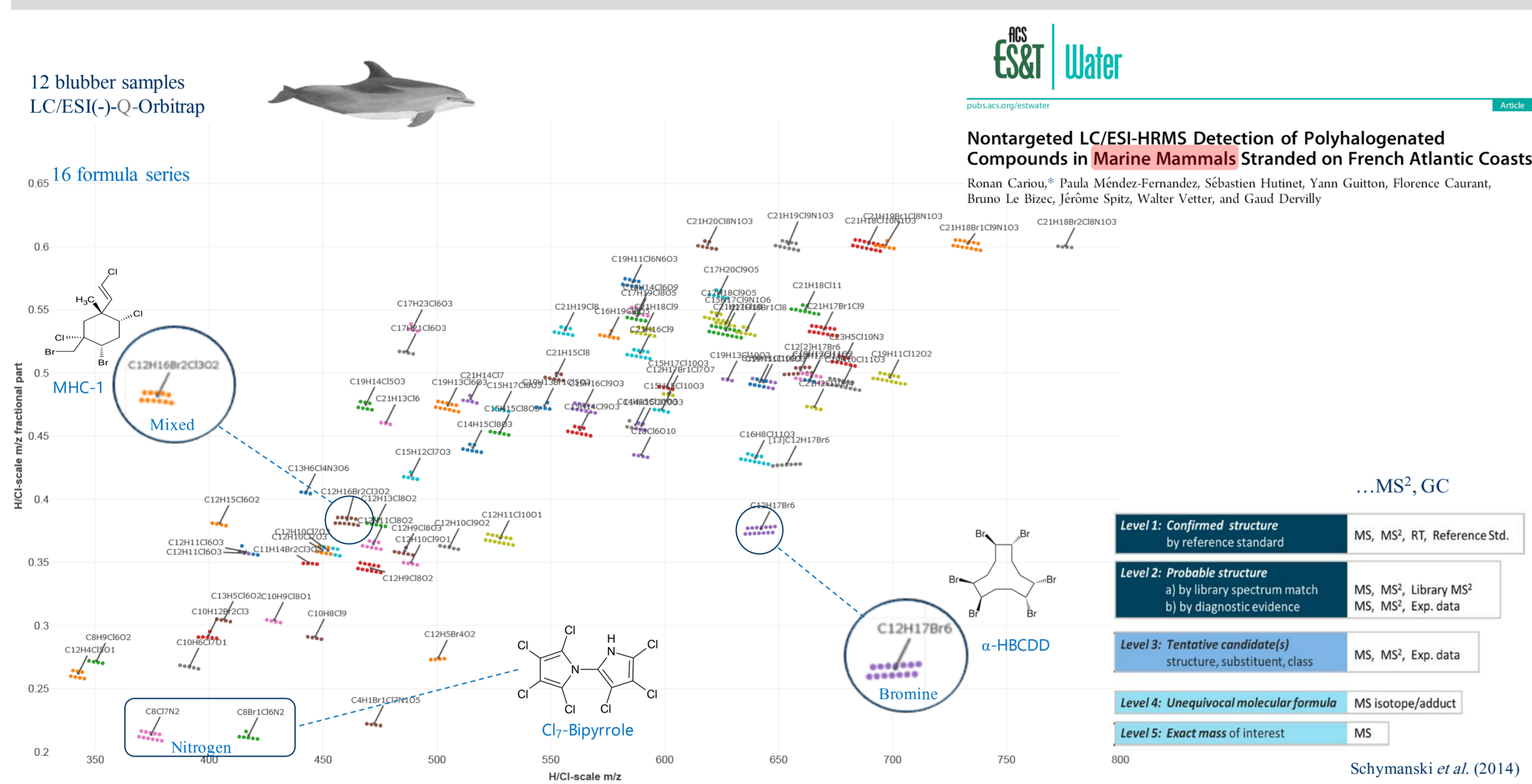
Introduction

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.

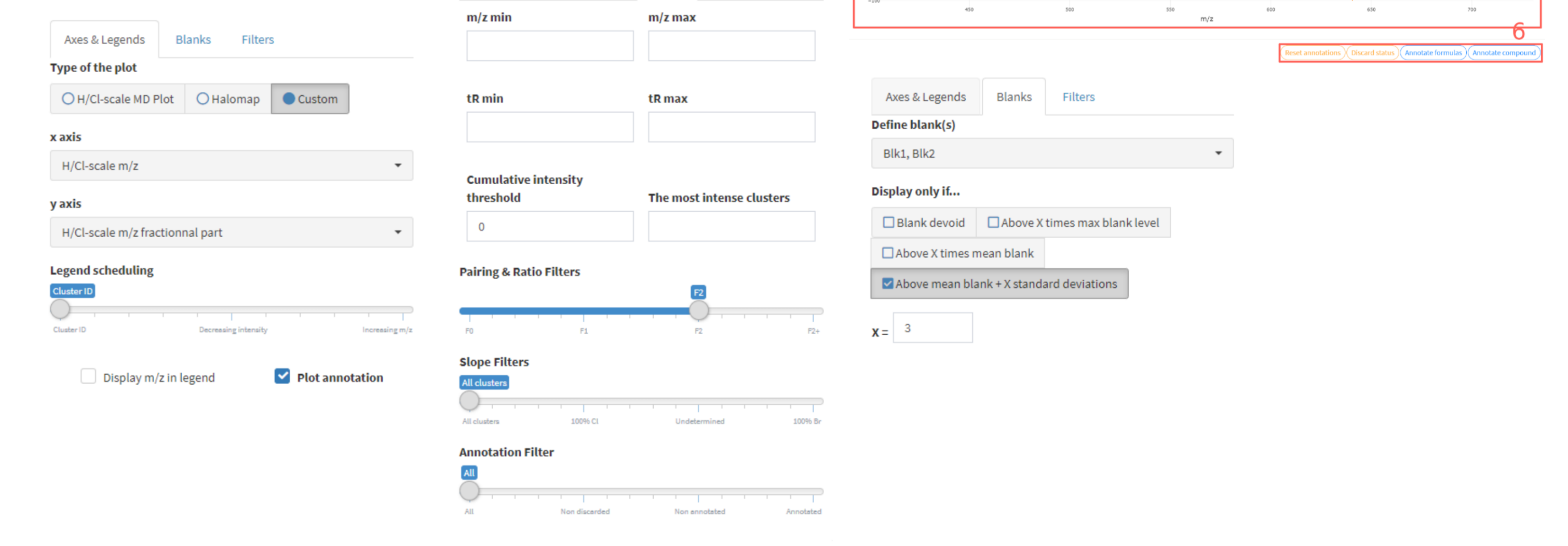
Workflow



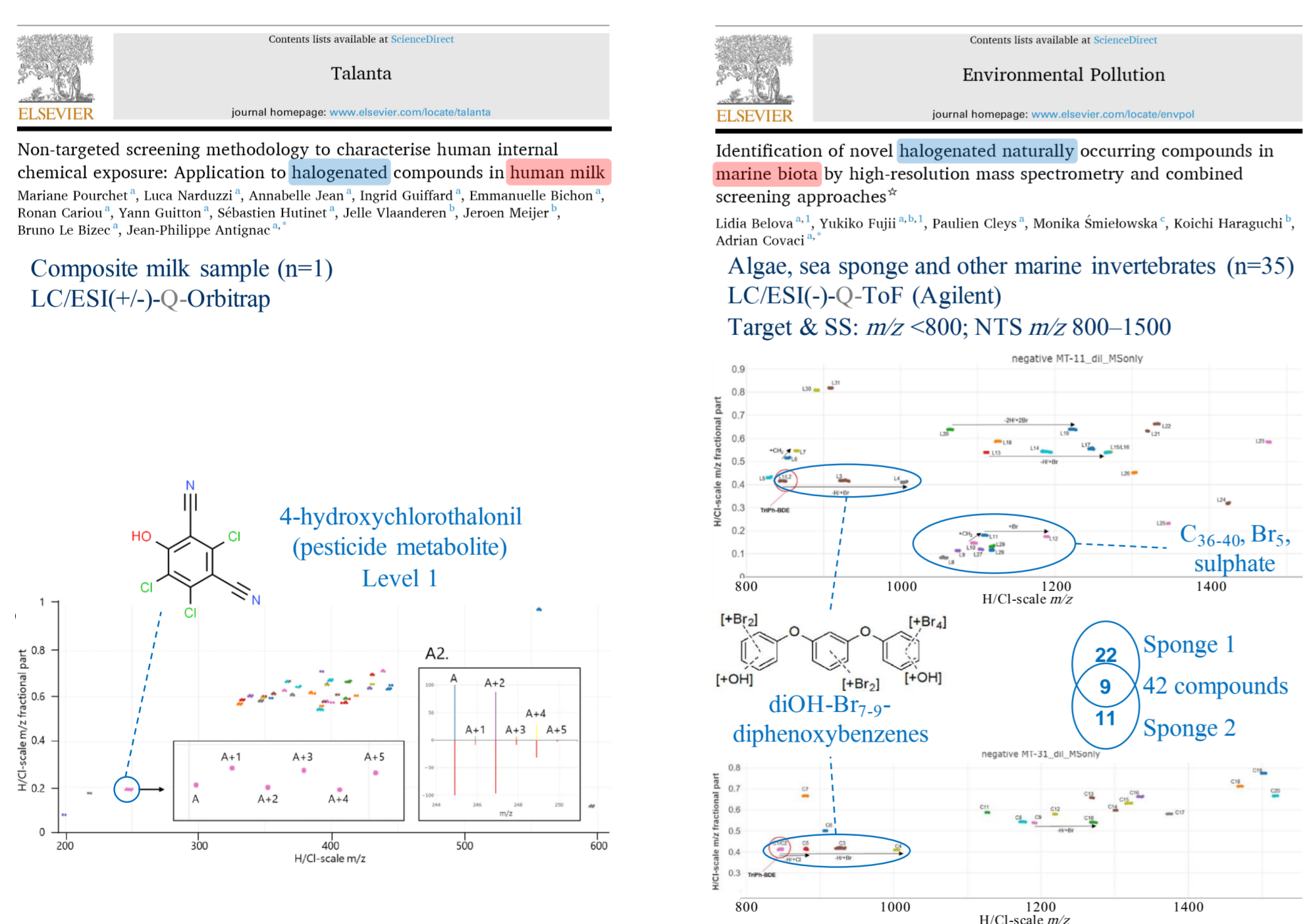
Application to marine mammal blubber



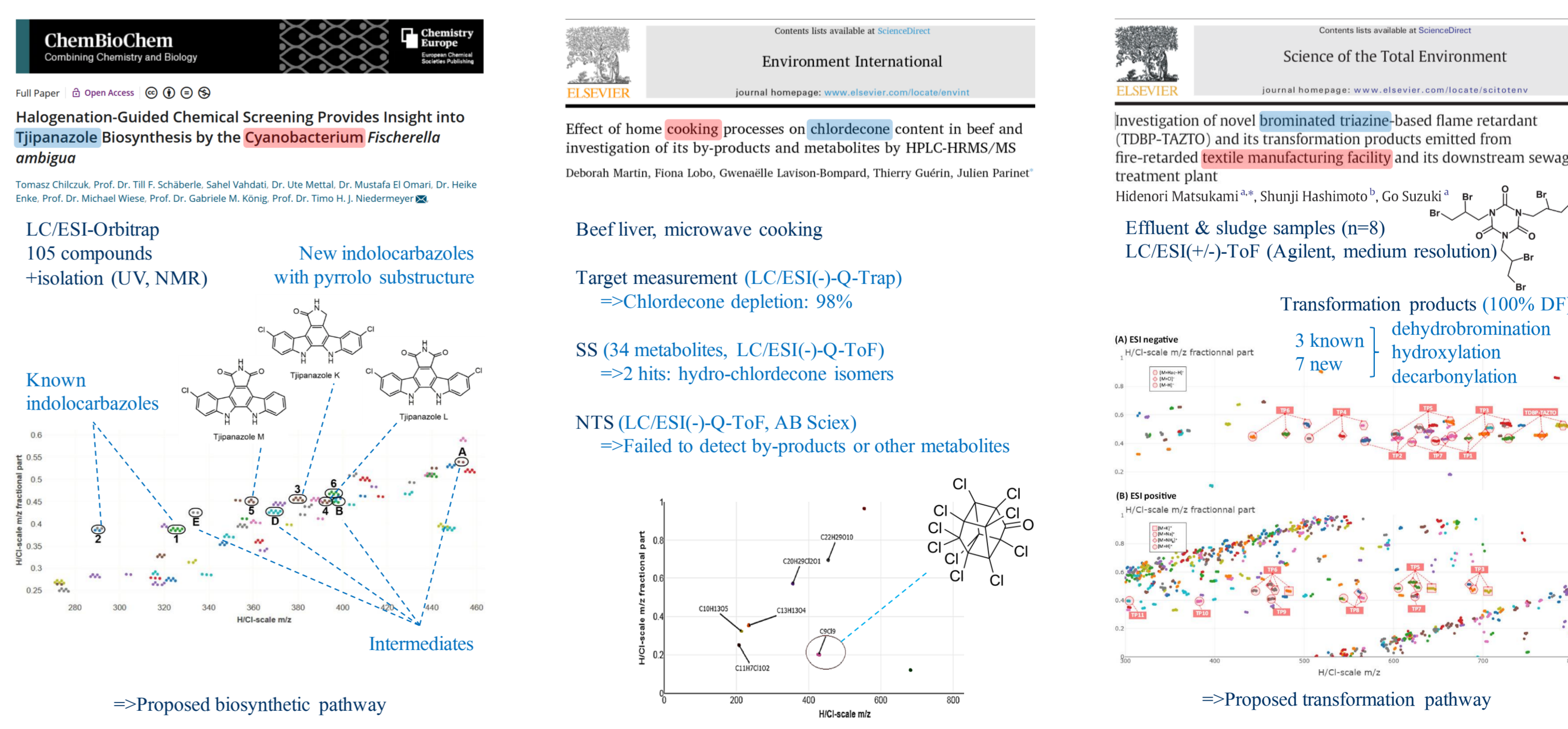
+ Display options



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.