



**HAL**  
open science

## Diving into the chemistry of sponge exo-metabolomes: contribution of brominated specialized metabolites

Morgane Mauduit, Stephane Greff, Thierry Pérez, Charlotte Simmler

### ► To cite this version:

Morgane Mauduit, Stephane Greff, Thierry Pérez, Charlotte Simmler. Diving into the chemistry of sponge exo-metabolomes: contribution of brominated specialized metabolites. Ecole thématique METABIODIVEX, Jun 2022, Aussois, France. 10.5281/zenodo.7254114 . hal-03857554

**HAL Id: hal-03857554**

**<https://hal.science/hal-03857554>**

Submitted on 17 Nov 2022

**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.



Distributed under a Creative Commons Attribution 4.0 International License



# Diving into the chemistry of sponge exo-metabolomes: contribution of brominated specialized metabolites

Morgane MAUDUIT<sup>1</sup>, Stéphane GREFF<sup>1</sup>, Thierry PEREZ<sup>1</sup>, Charlotte SIMMLER<sup>1</sup>

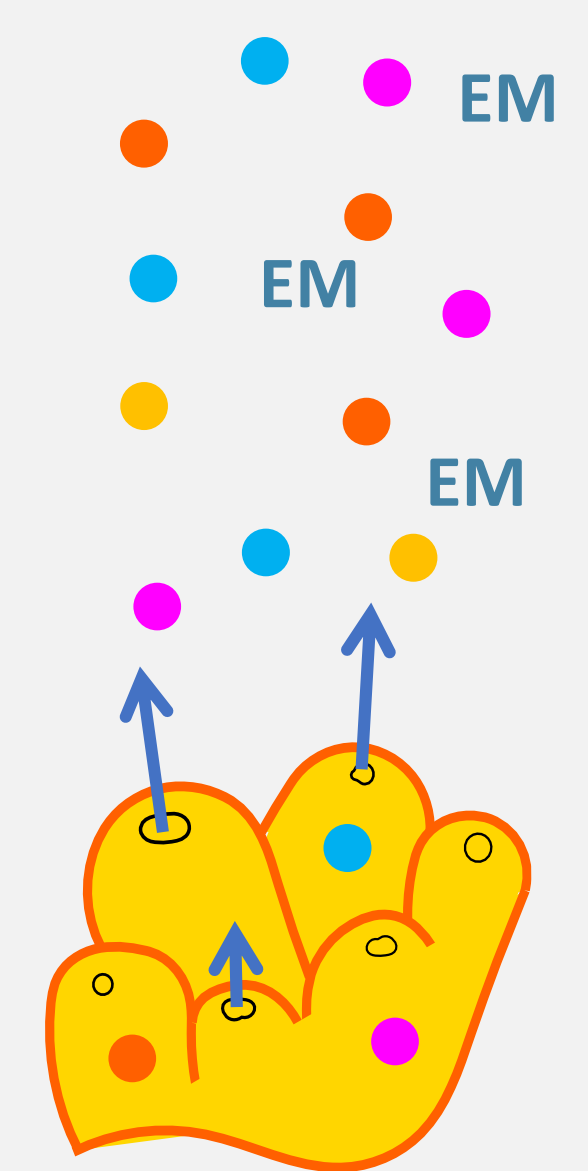
<sup>1</sup> Institut Méditerranéen de Biodiversité et d'Écologie Marine et Continentale, UMR 7263  
Endoume Marine Station, rue de la batterie des lions, 13007 Marseille  
(e-mail: [morgane.mauduit@imbe.fr](mailto:morgane.mauduit@imbe.fr))



## Context

- Sponges produce **structurally diverse specialized metabolites** known for their biological/pharmacological potentials.<sup>1,2</sup> In particular, the Mediterranean sponges *Aplysina cavernicola* and *Agelas oroides* produce **brominated** alkaloids with antimicrobial/anti-biofilm properties.<sup>3,4</sup>
- A few targeted studies, performed on Caribbean species from the same genus, reported that the most abundant brominated alkaloid (e.g. aerothionin, oroidin) were detected in the seawater surrounding the sponges (●●●).<sup>5,6</sup>
- Hence, such exo-metabolites (EM) could be collected from the seawater without destroying the sponge biomass.

EXO-METABOLOME



Chemical Diversity

METABOLOME

What is the proportion (diversity & quant.) of specialized metabolites released by *A. cavernicola* & *A. oroides* in their surroundings?



*Aplysina cavernicola* (Vacelet, 1959)



Bromotyrosine spiroisoxazoline alkaloids

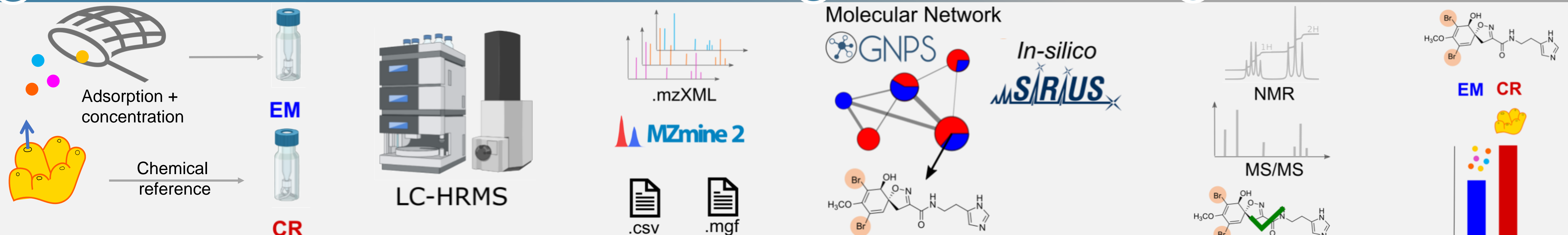


*Agelas oroides* (Schmidt, 1864)



Bromopyrrole alkaloids

## 1 Sample preparation MS<sup>2</sup> acquisition & processing 2 Annotation, Dereplication 3 Identification & Quantification



## Results

### 1 Exo-metabolites (EM) concentration

- Comparison of different polymeric resins → Solid phase selection according sponge chemistry
- Variation of the experiment duration
- Metabolite adsorption with/without stress

### 2 Chemical diversity of *A. cavernicola* EM

11.2 Br

88.8

Analysis of Mzmine extracted features MS isotopic pattern

Reproducibly detected → SIRIUS Chemical superclass Sirius score > 100

Lipids & lipid-like

- 11% of the total detected EM features were found to be **brominated** (structures with 2/4 Br) & could correspond to *A. cavernicola* specialized metabolites.
- 79% of the reproducibly detected EM features belong to the class of **lipids and lipid like molecules**.

### 3 Identification of brominated exo-metabolites

#### MS<sup>2</sup> based annotation & dereplication

FBMN : Bromotyrosine spiroisoxazoline

aerothionin

#### <sup>1</sup>H NMR spectrum of aerothionin (CD<sub>3</sub>OD, 600 MHz)

Isolation → Raw data → 1D/2D NMR + MS<sup>2</sup> Public DB (GNPS-ZENODO)

- A total of **6 characteristic brominated alkaloids** identified by MS and NMR analyses after purification were detected in the seawater, including aerothionin.
- All their MS and NMR data will be shared in open access database.

## Conclusions & Perspectives

- The present experimental and analytical workflow enable us to determine the proportion & identity of brominated exo-metabolites (EM) recovered from the seawater surrounding *A. cavernicola*. The same workflow was implemented with *A. oroides*. Quantitative analysis are in progress. Collectively, those EM are possibly released through the sponge metabolic activities & cellular turnover.<sup>7</sup>
- Such results will serve as a stepping stone to:
  - guide *in situ* field work to study the release of specialized metabolites by both sponge species
  - propose a valorisation of sponge chemical diversity without collecting their biomass

## References:

1. Carroll, A. R., et al. *Nat. Prod. Rep.* (2022) 2. Pawlik, J., et al. *Mar. Ecol. Prog. Ser.* 127, 183–194 (1995) 3. Peng, J., et al. *AlkaloidsChemBiol.* 61: 59–262 (2005) 4. Richards, J., et al. *Bioorg Med Chem Lett.* 18(15):4325–7 (2008) 5. Walker, R. P. et al. *Mar Biol* 88, 27–32 (1985), 6. Richelle-Maurer, E., et al. *Biochemical Systematics and Ecology* 31, 1073–1091, (2003) 7. de Goeij, J. M., et al. *Science* 342, 108–110 (2013)