

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

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

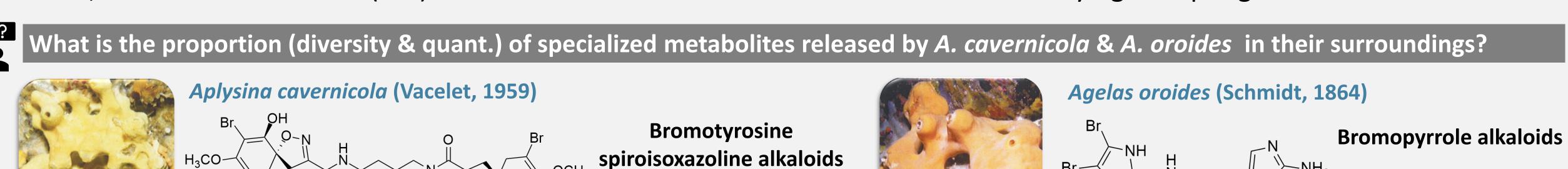
# Morgane MAUDUIT<sup>1</sup>, Stéphane GREFF<sup>1</sup>, Thierry PEREZ<sup>1</sup>, Charlotte SIMMLER<sup>1</sup>

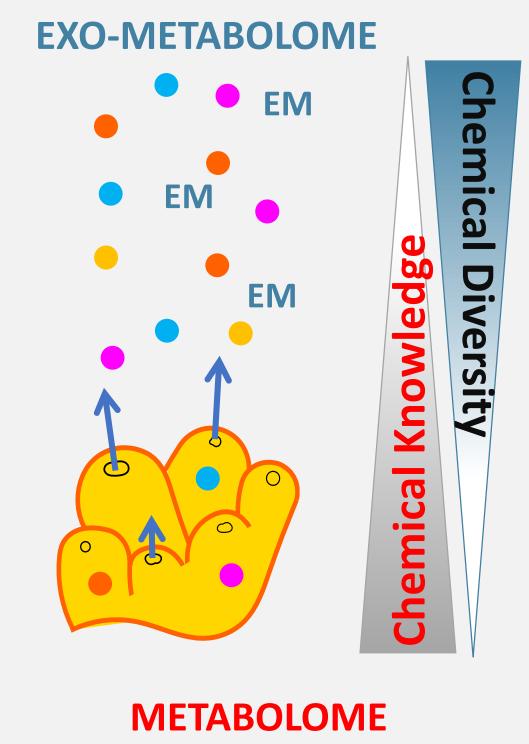
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### Context

- Sponges produce structurally diverse specialized metabolites known for their biological/pharmacological potentials. 1,2 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 (•••).5,6
- Hence, such exo-metabolites (EM) could be collected from the seawater without destroying the sponge biomass.





Sample preparation

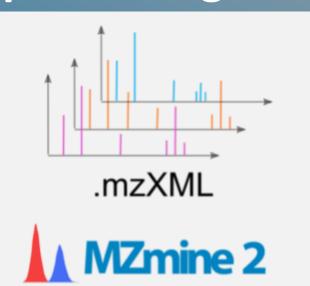
Chemical

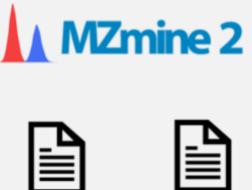
reference

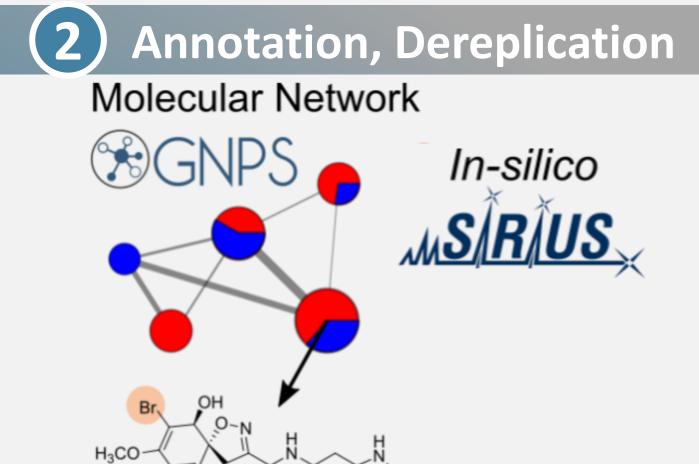
Adsorption +

concentration

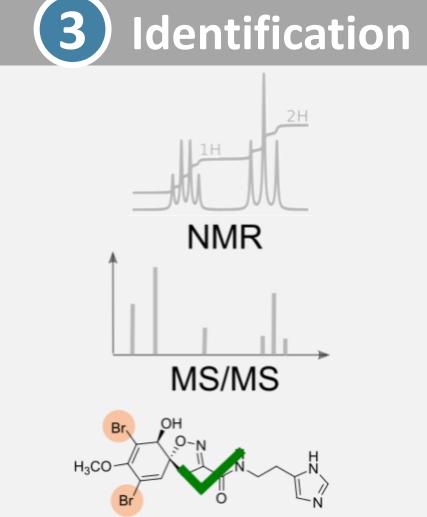
MS<sup>2</sup> acquisition & processing

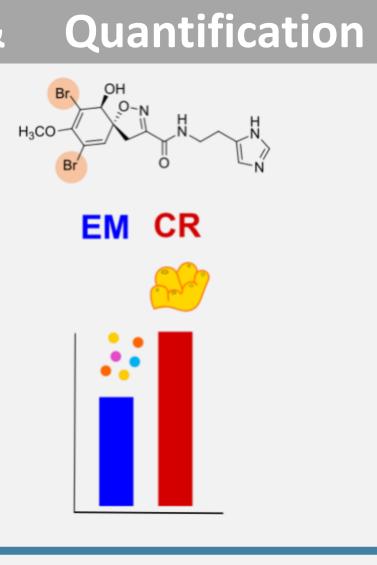






oroidin





Results

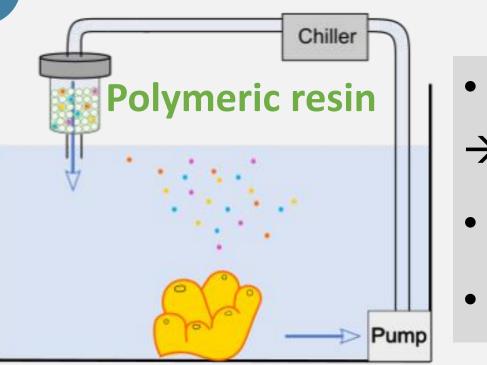
## **Exo-metabolites (EM) concentration**

aerothionin

EM

CR

НО



Comparison of different polymeric resins

LC-HRMS

→ Solid phase selection according sponge chemistry

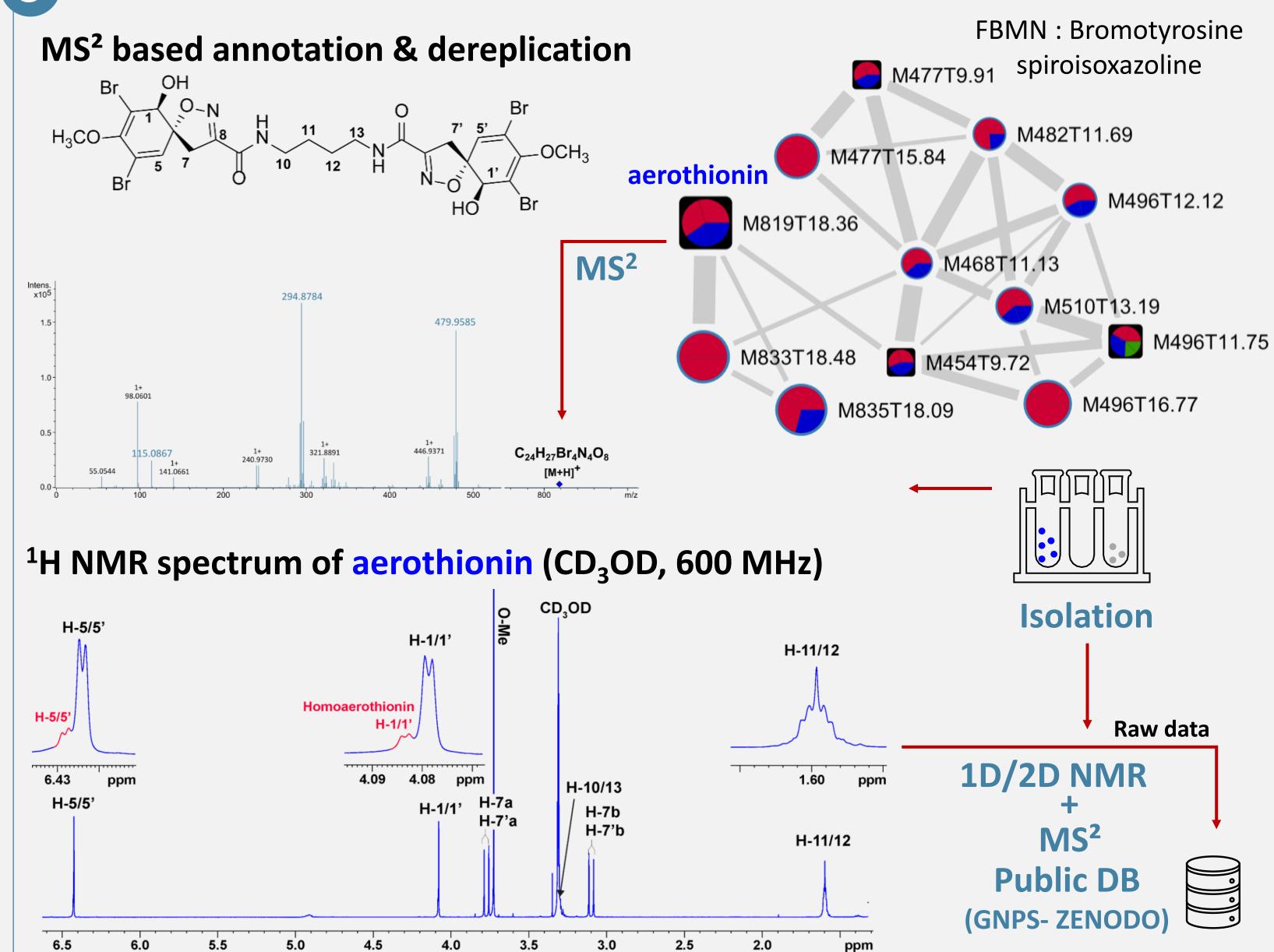
Variation of the experiment duration

- Metabolite adsorption with/without stress

# Chemical diversity of A. cavernicola EM 11.2 Analysis of Mzmine extracted features MS isotopic pattern 88.8 Reproducibly detected **Chemical superclass** E Lipids & lipid-like Sirius score > 100

- 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.

### Identification of brominated exo-metabolites



- 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. 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)









