

Targeted Metabolome Mining for Antimicrobial Peptides

Supervisor	Ass.-Prof. Mitja M. Zdouc , Division of Pharmacognosy
Topic	Data Mining, Metabolomics, Natural Products
Duration and type	6 Months (full-time), computational work only
Requirements	Bachelor in Pharmacy, Informatics, or similar
Language	English/German

Description

Microbial specialized metabolites impress with their chemical diversity and potent biological activities. Among these so-called **natural products (NPs)**, the class of **Ribosomally Synthesized and Post Translationally Modified Peptides (RiPPs)** are known for their strong antimicrobial activities [1]. However, RiPPs are usually subject to strong transcriptional regulation, resulting in low production titers, complicating their **detection**. Therefore, **targeted metabolome mining** is needed to effectively detect RiPP NPs, and **rational prioritization** of the putative candidates is key for successful follow-up isolation and investigation.

In this project, you will start with existing liquid chromatography tandem mass spectrometry (**LC-MS/MS**) data of bacterial isolates. You will use metabolome mining techniques to **interrogate the data for putative RiPPs**, using the programs mzmine [2] and FERMO [3]. Once putative RiPP candidates are identified, you will perform **rational prioritization** by integrating **bioactivity assay data** and **cultivation conditions**. The most promising isolation candidates will undergo **genome sequencing**, and you will pair metabolomics and genomics data to link genotype to phenotype. Your work will inform **follow-up isolation and characterization** of these RiPPs, with the potential to discover new antimicrobials usable in medicine and agriculture.



Learning outcomes

At the end of this Master thesis, you will be able to:

- **Process** and **analyze** LC-MS/MS data, using metabolome mining techniques.
- **Apply** prioritization techniques and **interpret** and **integrate** genome mining information.
- **Interpret** results, summarize findings, and **document** your work using FAIR data principles [4]
- **Present** findings in word and text and **understand** the manuscript writing process.

How to apply

Please contact Ass.-Prof. Mitja Zdouc via E-Mail (mitja.zdouc@univie.ac.at), indicating the progress of your studies, your preferred starting date, and if you fulfill the requirement criteria. Please include a brief statement about your research interest, why you would like to work on this project, any prior knowledge related to the topic, as well as preferred working style and supervision expectations. Applicants will be invited for a brief interview where the project will be discussed in detail.

References:

- 1 Arnison et al. 2013 Nat Prod Rep DOI: [10.1039/C2NP20085F](https://doi.org/10.1039/C2NP20085F)
- 2 Zdouc et al. 2025 bioRxiv DOI: [10.1101/2022.12.21.521422](https://doi.org/10.1101/2022.12.21.521422)
- 3 Schmid et al. 2023 Nat Biotech DOI: [10.1038/s41587-023-01690-2](https://doi.org/10.1038/s41587-023-01690-2)
- 4 Wilkinson et al. 2015 Sci Data DOI: [10.1038/sdata.2016.18](https://doi.org/10.1038/sdata.2016.18)