



Master project 2021-2022

Personal Information

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Institution	IBEC
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Group	Signal and Information Processing for Sensing Systems

Project

Web development & bioinformatic tools

Project Title:

Comparison of workflows for the analysis of LCMS data in R

Keywords:

Computational Metabolomics, Biomarker Discovery, Machine Learning, Full Workflows

Summary:

There is a variety of tools for the analysis of LCMS data in computational metabolomics. The full workflow considers raw signal preprocessing plus machine learning aiming to biomarker discovery. Using public datasets the student will do a critical analysis of the current tools to identify potential room for improvement. Current open source solutions will be benchmarked against the tool currently being developed in house.

References:

Stanstrup, J., Broeckling, C. D., Helmus, R., Hoffmann, N., Mathé, E., Naake, T., Nicolotti, L., Peters, K., Rainer, J., Salek, R. M., Schulze, T., Schymanski, E. L., Stravs, M. A., Thévenot, E. A., Treutler, H., Weber, R., Willighagen, E., Witting, M., & Neumann, S. (2019). The metaRbolomics Toolbox in Bioconductor and beyond. *Metabolites*, 9(10), 200. <https://doi.org/10.3390/metabo9100200>

Expected skills::

R programming

Possibility of funding::

No

Possible continuity with PhD: :

To be discussed

