Universitat Pompeu Fabra Barcelona

Master in Bioinformatics for Health Sciences

Master project 2024-2025

Personal Information

Supervisor	Santiago Marco
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Institution	IBEC
Website	https://ibecbarcelona.eu/sensingsys
Group	Signal and Information Processing for Sensing Systems

Project

Web development & bioinformatic tools

Project Title:

Full workflows for untargeted metabolomics with Gas Chromatography_Ion Mobility Spectrometry

Keywords:

metabolomics, biomarker discovery, machine learning, feature selection, feature extraction

Summary:

Untargeted metabolomics is increasingly recognized for its potential in personalized medicine, with advanced data analysis playing a critical role. This project will address the challenges of developing reliable predictive models due to biological and instrumental variance. We will address the analytical process for handling data from chemical instrumentation (in this case gas chromatography-ion mobility spectrometry) used in biofluid analysis, focusing on feature extraction challenges and the creation of machine learning-based predictive models, especially for biomarker discovery through feature selection.

References:

Oller-Moreno, S., Mallafré-Muro, C., Fernandez, L., Caballero, E., Blanco, A., Gumà, J., ... & Pardo, A. (2023). GCIMS: An R package for untargeted gas chromatography–Ion mobility spectrometry data processing. Chemometrics and Intelligent Laboratory Systems, 241, 104938.

Expected skills:

R programming, Machine Learning, Statistics

Possibility of funding:

No

Possible continuity with PhD:

To be discussed