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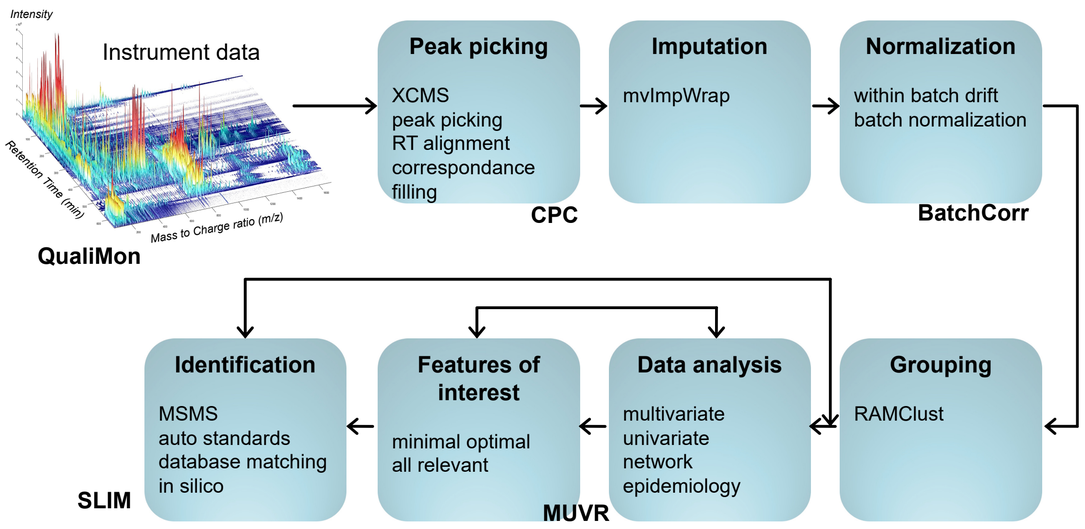
A Modular Bioinformatics Pipeline for High Throughput Analysis at the SciLifeLab Metabolomics Platform



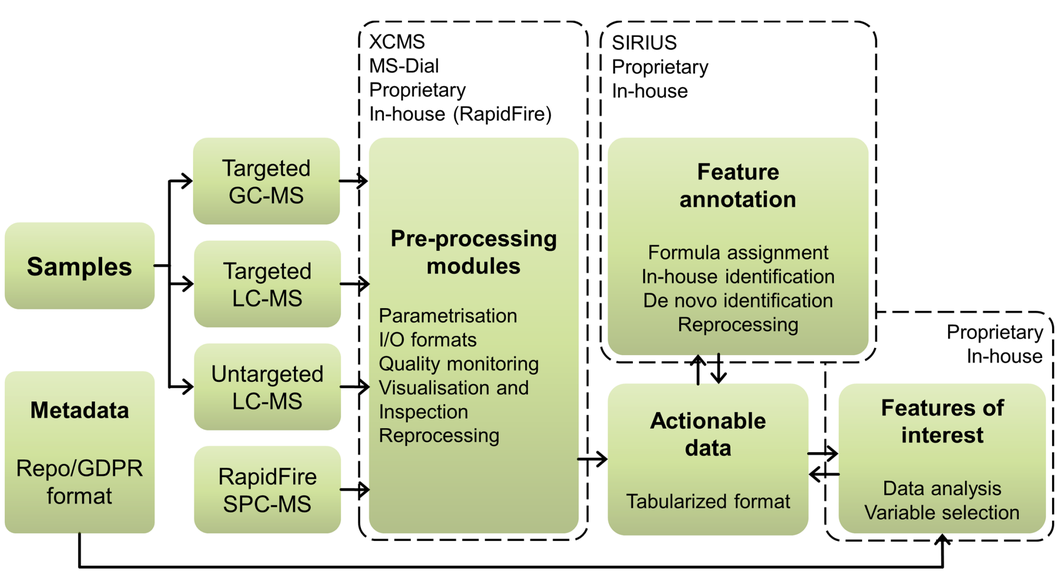
Overview of the (pre)-processing workflow

High-throughput analysis

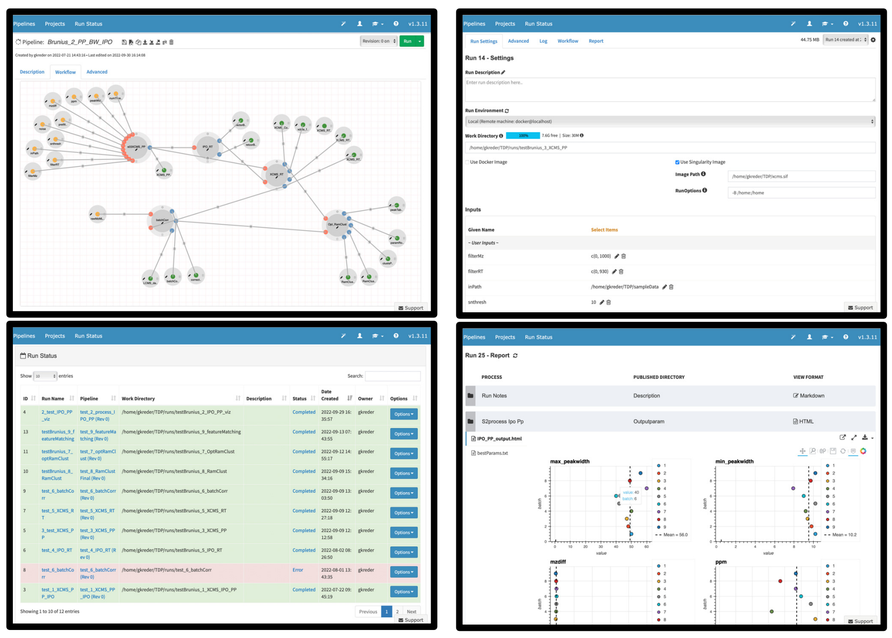
Computational workflows, from data pre-processing to final metabolite annotation, have been developed in the SciLifeLab Platform for Mass-spectrometry-based metabolomics and exposomics.

Current tools are built in different software environments (proprietary and open source).

Our aim is to combine them into more effective, easy-to-use pipelines for higher throughput.



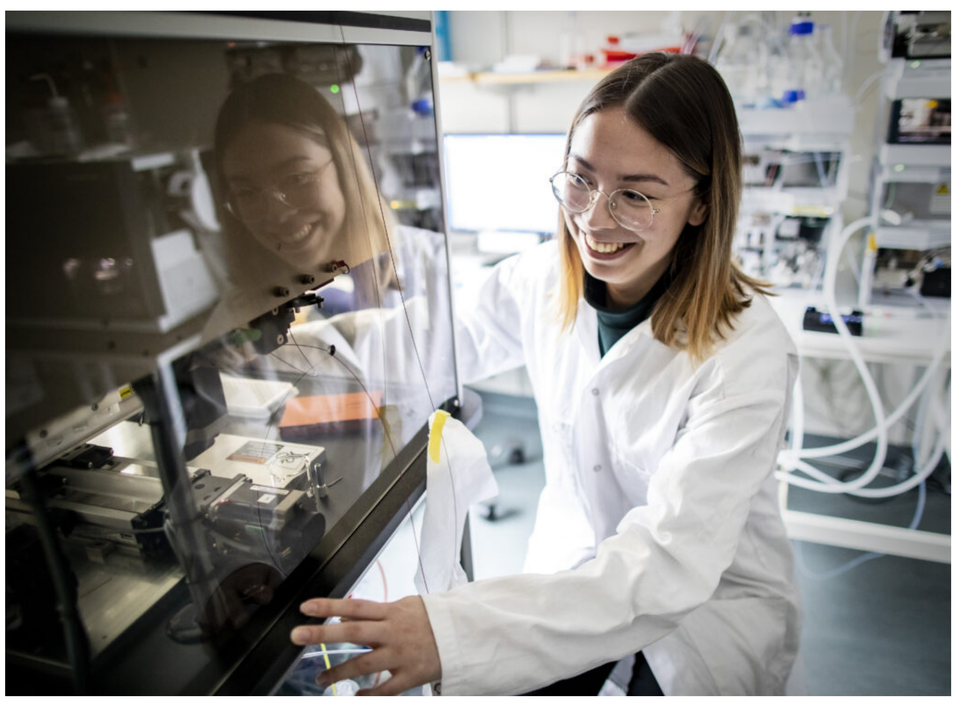
Design of a modular pipeline for the Metabolomics and Exposomics Platform



Pilot version of pipeline developed in DolphinNext and implemented at CMSI enabling interactive pipeline creation, version editing, run management, and output visualization

Explore and reuse living data deliveries with full FAIRness

Implementing this pre-processing strategy will facilitate and improve bioinformatics throughput, which is the rate-limiting step in the platform. In particular for larger scale studies, thus providing large-scale molecular data for deep learning (DL) and artificial intelligence (AI) in data-driven Life Science research.



SciLifeLab Metabolomics platform member using the Agilent RapidFire 400, designed for extreme throughput using solid phase extraction – mass spectrometry. The system allows sample analysis with cycle times of approximately 10 s.

RapidFire – mass spectrometry

Ultra high-throughput screening

A new targeted method has been developed that enables rapid data extraction, matching the instrument cycle time of 10 s per sample.

This development provides potential for analysis of up to 60 000 samples per week and instrument, enabling next generation large-scale data generation.

SciLifeLab has been created by the coordinated effort of four universities in Stockholm and Uppsala: Stockholm University, the Karolinska Institutet, KTH Royal Institute of Technology and Uppsala University.