

Metabolomics Core Facility provides ready to use data exploration with MetaboScape

Core facilities in academic institutions provide services and instrument access to research labs that by themselves lack the expertise and/or resources to perform metabolomics experiments.

This involves working with tens to hundreds of users with greatly varying levels of knowledge in metabolomics and analytical technology. Whilst designing metabolomics experiments and acquiring data is typically performed by specialized and trained staff, successful data processing, in particular for untargeted metabolomics, requires knowledge of the experimental system and the experimental design. Ideally, experts from the core facility and users from the research labs review the data together.



MetaboScape® is designed as an all-in-one software solution that includes feature extraction from raw data, statistical analysis, feature identification, and data visualization. The software is accessible even to inexperienced users and robust default settings enable them to generate reliable results. In addition, the core facility has defined optimized parameter sets for custom LC-MS methods (e.g. HILIC). These custom settings can be shared with users, who can select them in the client. Using these expert-approved processing settings ensures high data quality and reproducibility.

Access to processing methods and results is controlled through MetaboScape's built-in user management. This drastically facilitates collaborative data analysis.

Dr. Jörg Büscher, *Head of Metabolomics Facility, MPI of Immunobiology and Epigenetics, Freiburg, Germany, explains:*

"Users can easily install the MetaboScape Client on their local workstations. The MetaboScape Server sited in the same network is automatically detected so that the client connections and the server work seamlessly."



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Challenges

The multi-user environment in core facilities poses several challenges:

- Typically, the core facility experts must spend time to explain the software workflow and utilization (often comprising several independent software packages) to tens or hundreds of, often single time, users.
- The common single site license model for many software packages allows for single user access only.
- Experts from the core facility and their researchers want to jointly process data and review results.

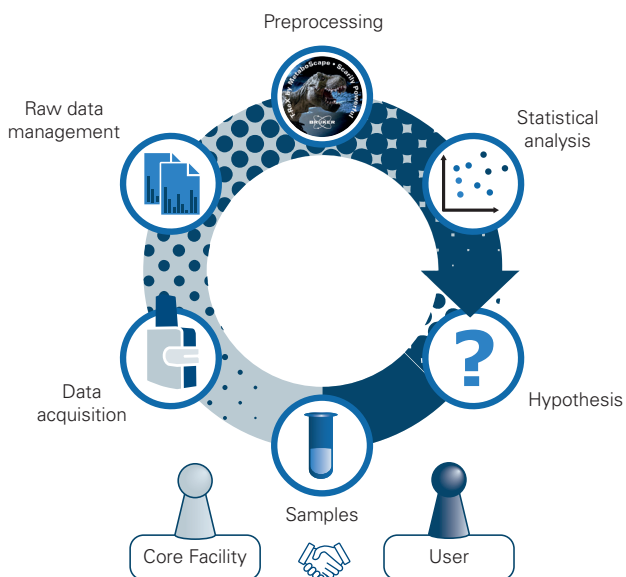


Figure 1: Users approach core facilities with a hypothesis to be tested and a batch of samples. Core facilities provide the tools and the knowledge to acquire MS data of these samples and offer their experience with data processing and statistical analysis to the users.

Solution

The MetaboScope all-in-one client server workflow solutions was developed for a collaborative research environment. Experts in fields ranging from metabolomics, lipidomics, phenomics, foodomics, exposomics and environmental contaminants can work on a shared data set together with users who have a different field of expertise. This design makes MetaboScope particularly suitable for core facilities servicing their local scientific community.

- Data processing, annotation, and evaluation workflows in MetaboScope are optimized for ease of use, so the core facility experts do not have to spend significant time explaining the software to users.
 - Optimized parameter sets for common workflows can be shared by the core facility experts with their users.
- Client server architecture enables multiple users to evaluate their data at the same time.
- The user and project management in MetaboScope enables core facility experts and researchers to jointly preform processing on the same data set and subsequently review results.

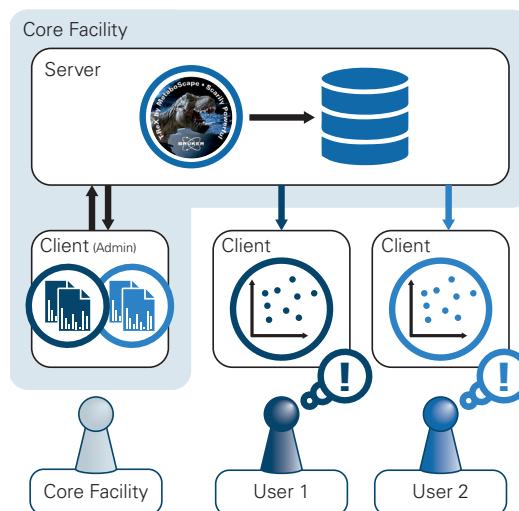


Figure 2: The MetaboScope client server architecture allows core facilities to make processed data accessible to the respective users. Both users and core facility members access the shared projects with the interactive client software in a collaborative fashion.

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