Metabolomics Core Facility provides ready to use data exploration with MetaboScape

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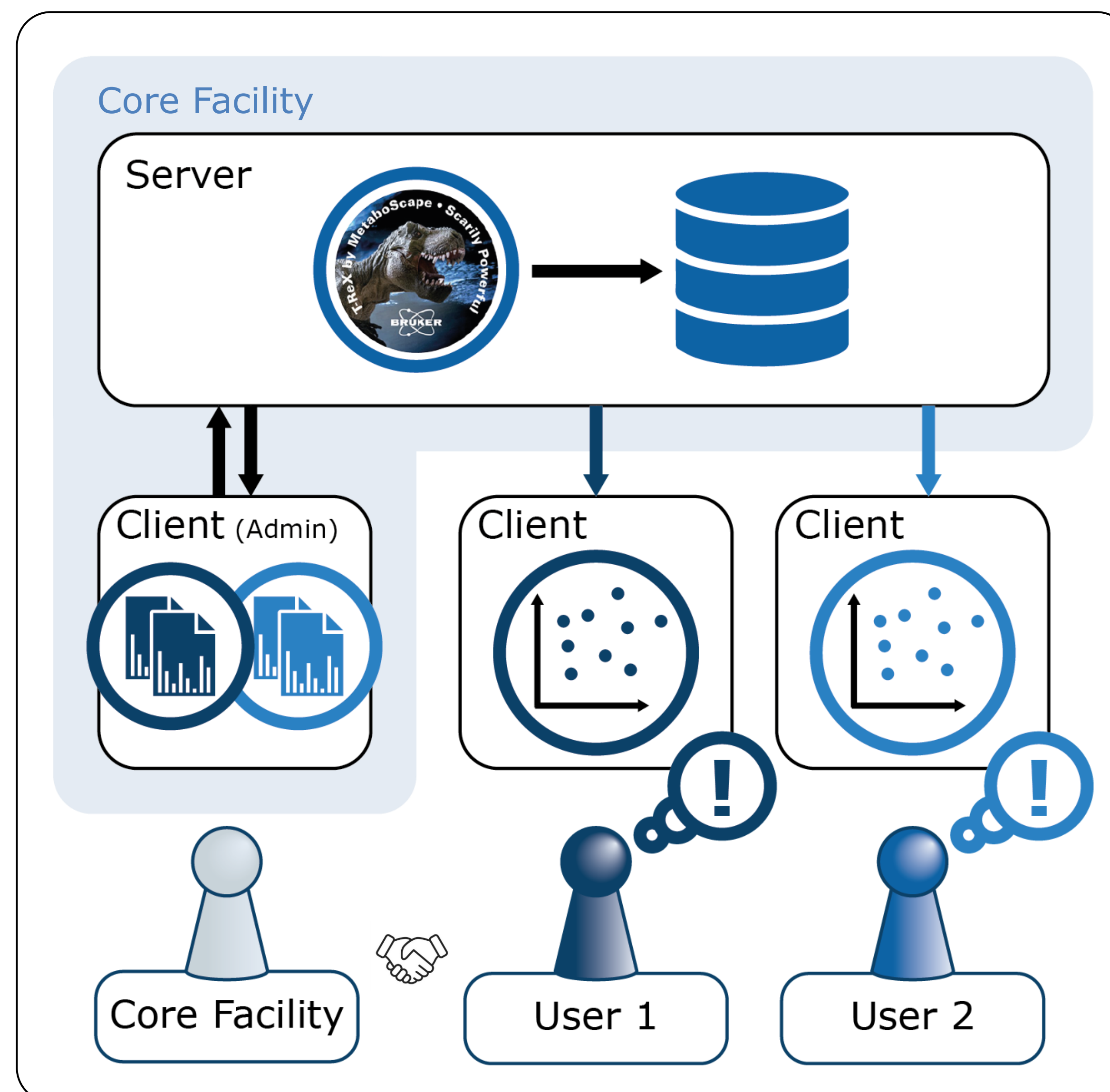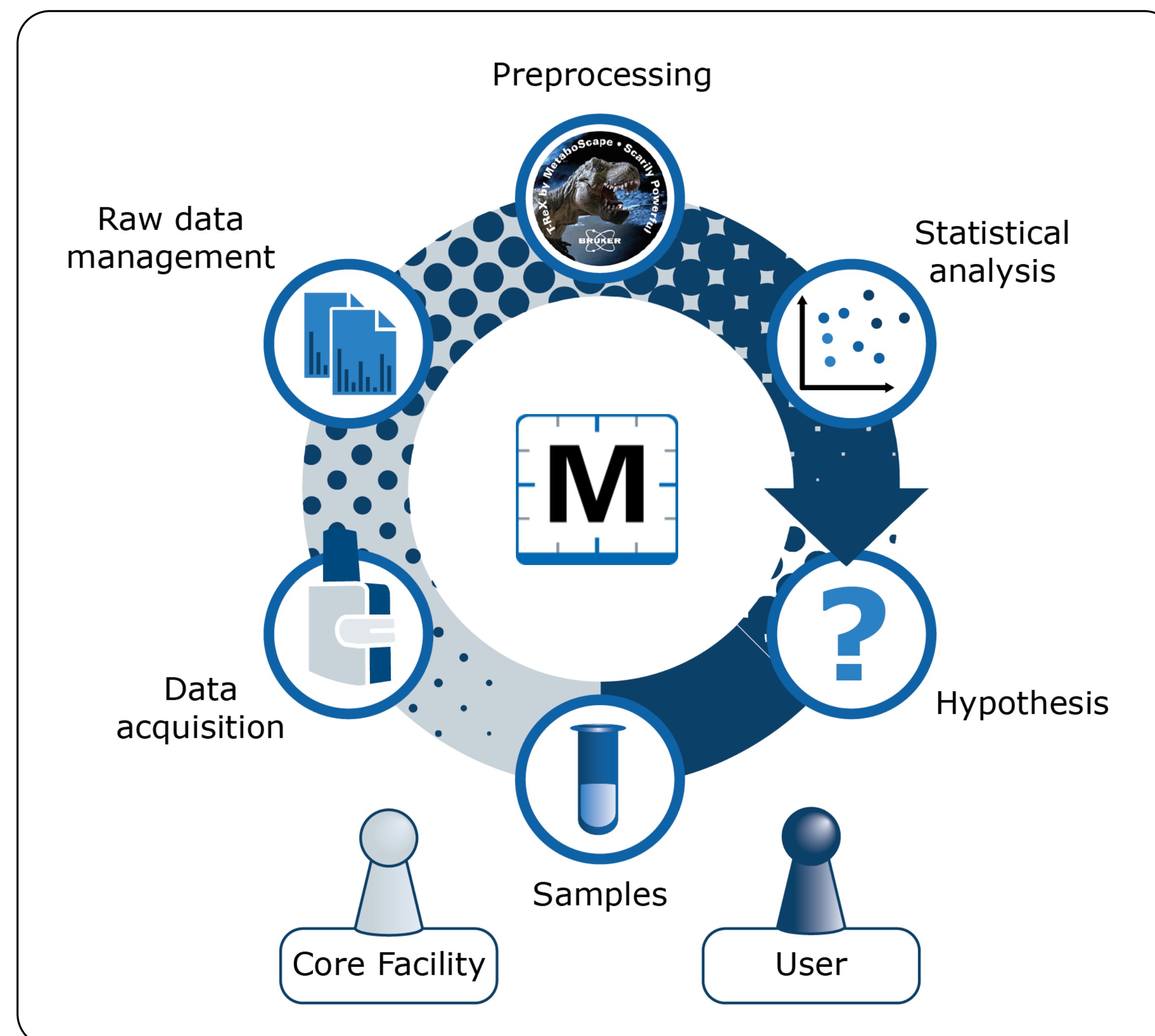[2]Bruker Daltonics GmbH & Co. KG, 28359 Bremen, Germany

Introduction

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.

Challenges

The situation described poses several challenges for the core facility members as well as their researchers:

- 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.

Solution

The MetaboScape 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 and can work together with users who have a different field of expertise on the same data. This design makes MetaboScape particularly suitable for core facilities servicing their local scientific community.

- Data processing, annotation, and evaluation workflows in MetaboScape 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 MetaboScape enables core facility experts and researchers to jointly preform processing on the same data set and subsequently review results.

At the Core Facility

- 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.

- The Core Facility can define 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 Core Facility-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.

Provide tailored methods for simple but consistent workflows

Core Facilities may process Feature Tables for their Users as a service. Additionally, they can design tailored processing methods and provide them as defaults to Users or User Groups.

Users get access to already processed Feature Tables, but may also build upon defaults created by the Core Facility and reprocess results.

Core Facilities can provide annotation methods most suitable for specific research areas.

Users can easily select the most suitable annotation methods and are only one click away from their annotated Feature Tables.

Sharing access to specific projects allows the Core Facility and Users to put their heads together to finally derive biological knowledge from their results.

MetaboScape