What’s new in MetaboScape® 2026

One integrated solution for processing and interpreting of MS based non-targeted Metabolomics, Lipidomics and Phenomics

Outline

01 Enhanced **T-ReX 4D** Processing Methods for **timsMetabo**

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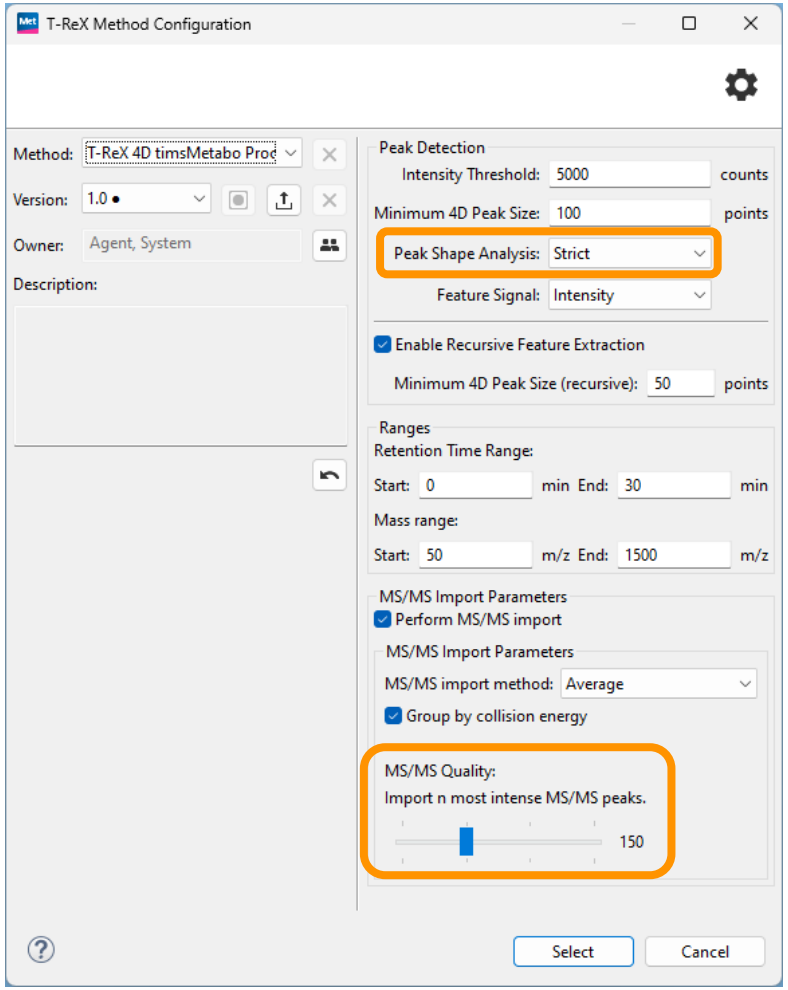
08 Improved Configuration Interface for Lipid Species Annotation

09 Fit Score and Reverse Fit Score Added for Spectral Library Matching

Enhanced T-ReX 4D Algorithms for timsMetabo

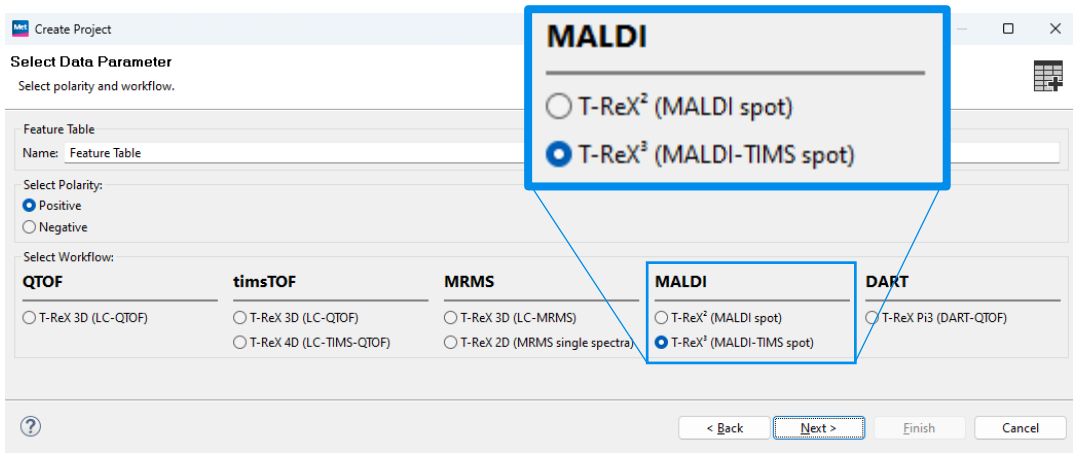
MetaboScape 2026 introduces new default processing methods for LC-TIMS-MoRE data from timsMetabo.

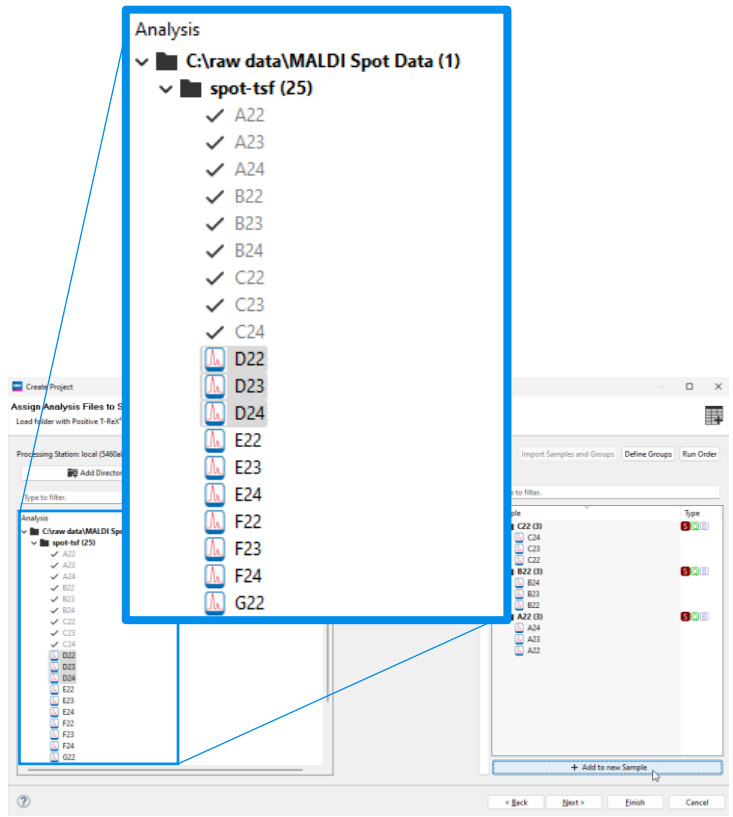
Leverage its high sensitivity and set your demands to peak quality higher, with the new parameter for strict peak shape analysis. Additionally, accelerate your data processing and interpretation by focusing on the most intense fragment peaks.



New T-ReX² and T-ReX³ Workflows for MALDI Spot Analysis

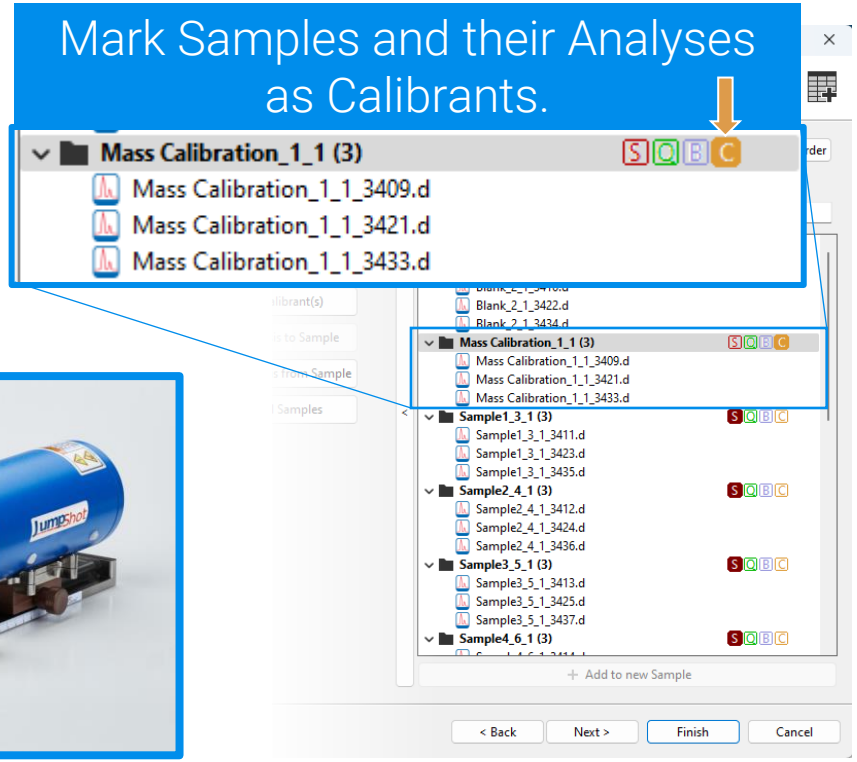
Dedicated processing workflows for MALDI-MS and MALDI-TIMS-MS data, supporting high-throughput spatial metabolomics with and without ion mobility separation.

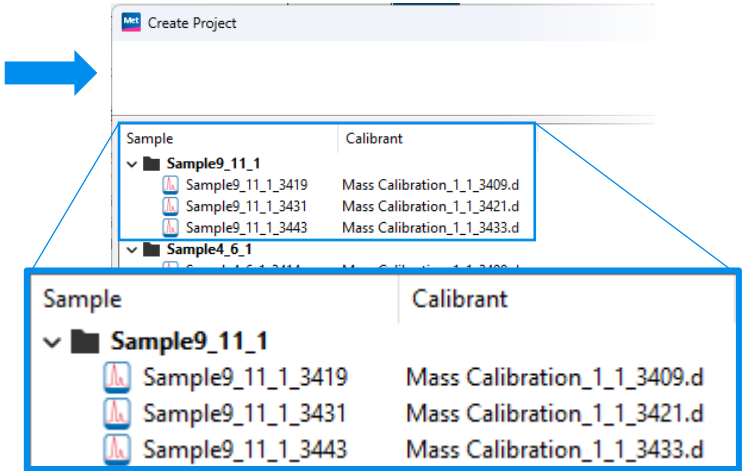




New T-ReX Pi3 Workflow for DART Processing with External Calibration

Specialized workflow for Direct Analysis in Real Time (DART) mass spectrometry, now supporting external calibration for enhanced mass accuracy and reproducibility.



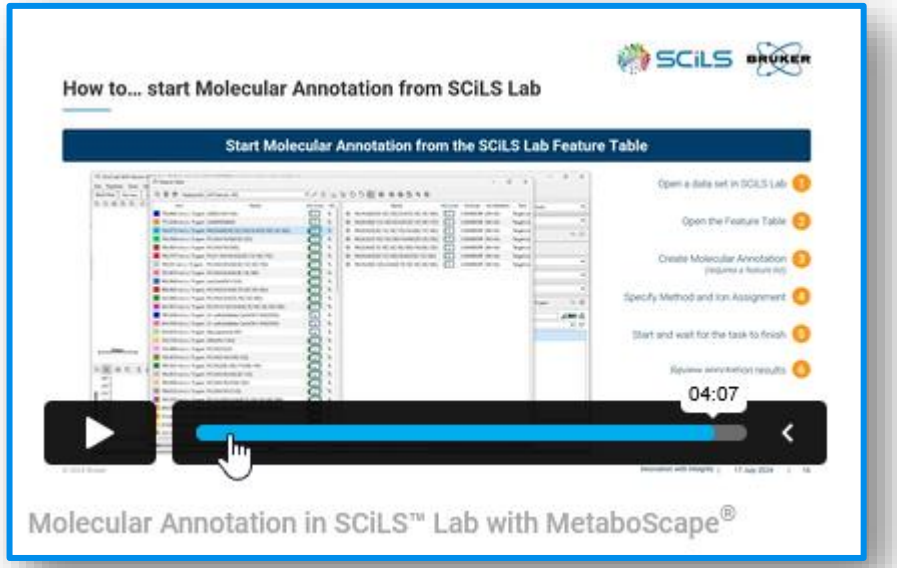


The relation of experimental samples to external calibrants is automatically established, but can be revised manually.

MALDI-Imaging Data Processing Transitioned to SCiLS-Lab

SCiLS Lab ❤ MetaboScape

2023b		T-ReX Feature Finding for Imaging data can be performed directly in SCiLS Lab.
2024a	2023b	SCiLS Lab and MetaboScape can be connected, unlocking the first of MetaboScape's annotation tools from within SCiLS Lab for MS1 annotation.
2025a	2023b 2025	SCiLS Lab introduces an iprm-PASEF workflow, and the MS/MS information can be subjected to annotation with MetaboScape: Target List w/ associated Spectral Library Rule-based Lipid Species annotation
2026a	2025b	Molecular Formula generation with SmartFormula
	2026	Transition of Imaging data processing from MetaboScape to SCiLS Lab is finalized. Imaging data processing in MetaboScape is obsolete.



Click here for a video tutorial on Molecular Annotation in SCiLS Lab with MetaboScape.

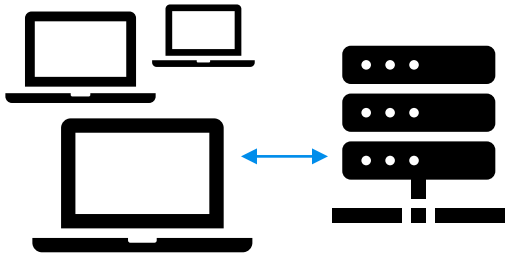
Remote Raw Data Processing via Networked Node

To support scalable and efficient data analysis, MetaboScape 2026 now allows processing on dedicated machines, offering greater flexibility in hardware resource management.

MOBILE

- Server
- Client
- Raw Data
- Processing

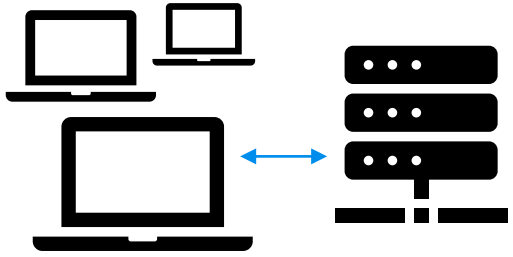
DEDICATED SERVER & PROCESSING ON CLIENTS



- Client(s)
- Raw Data
- Processing

- Server

DEDICATED SERVER & PROCESSING ON SERVER



- Client(s)

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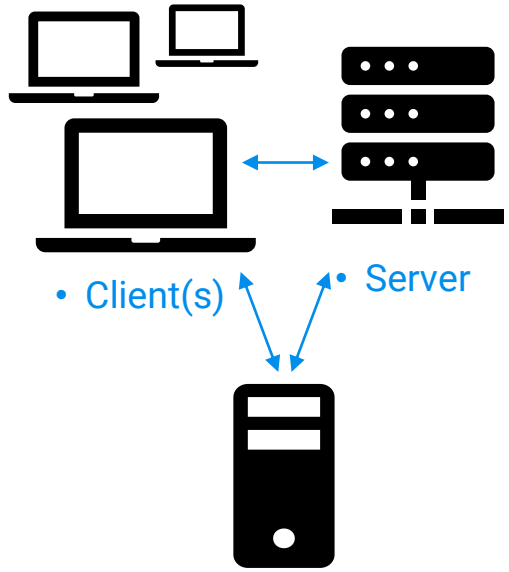

- Client(s)
- Server

- Raw Data
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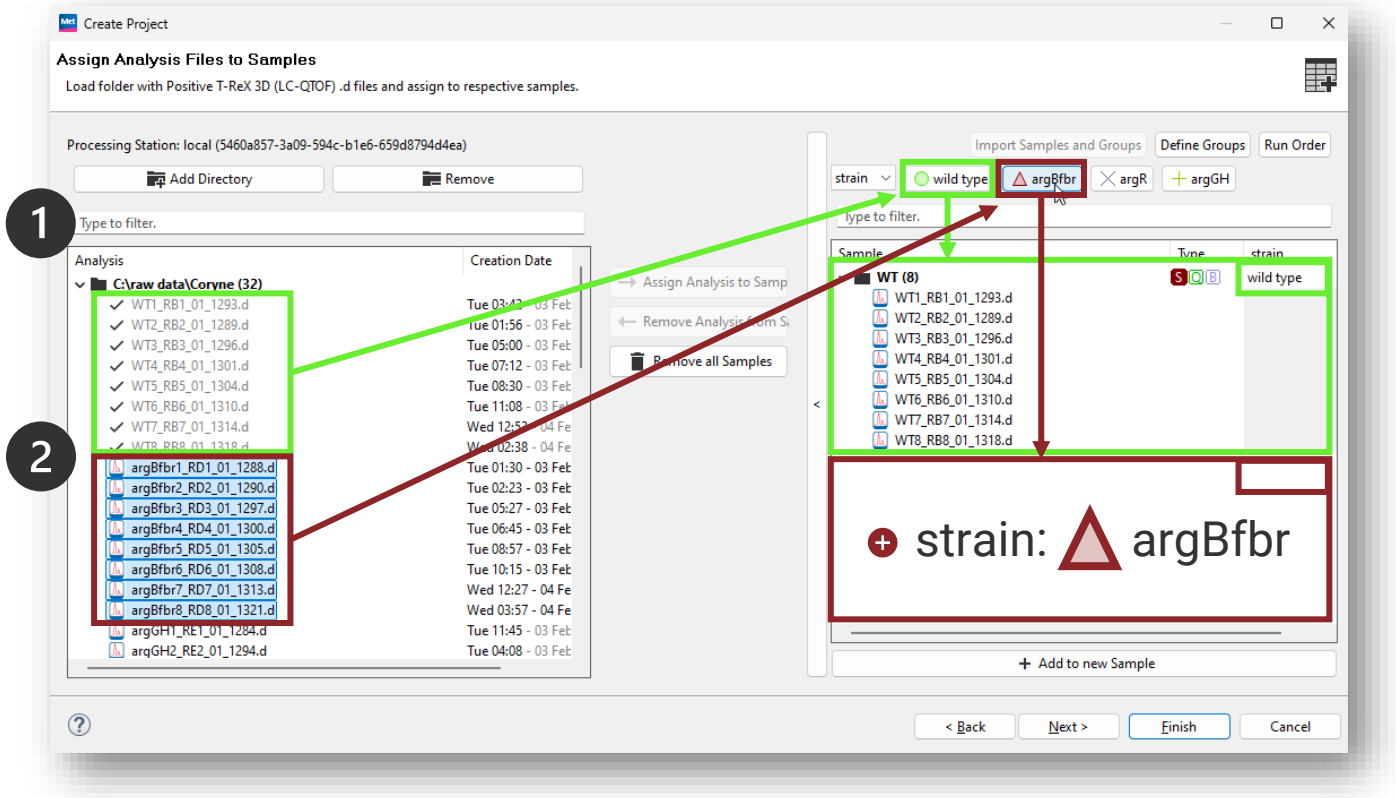
Refined User Interface for Sample and Analysis Setup

Streamlined UI components for intuitive configuration of sample tables and experimental designs, enhancing usability and reducing setup time.

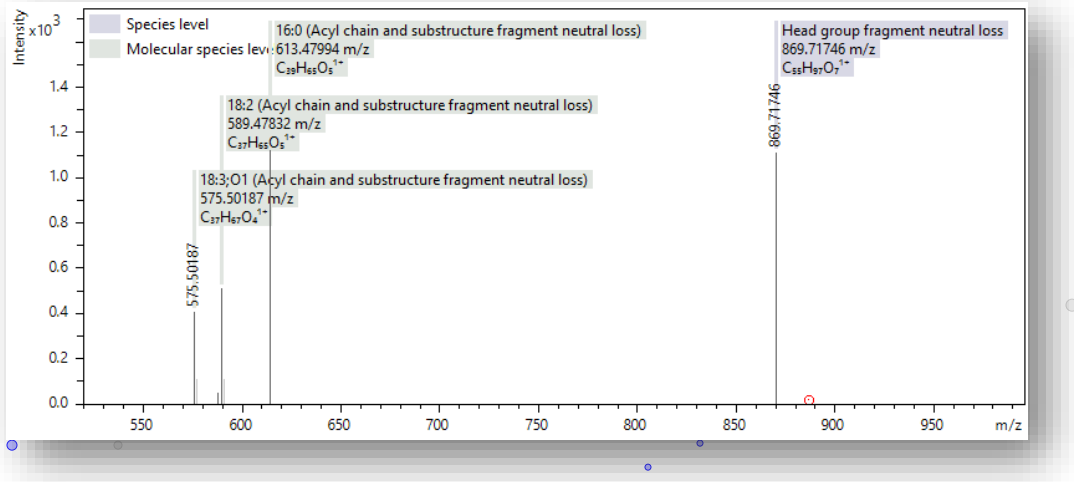


1. Use the filters for Analyses and Samples, to consolidate based on common identifiers in their names.

2. After defining your Groups and Attributes, select Analyses on the left and use the Attribute buttons to quickly create Samples, assigned to that attribute.

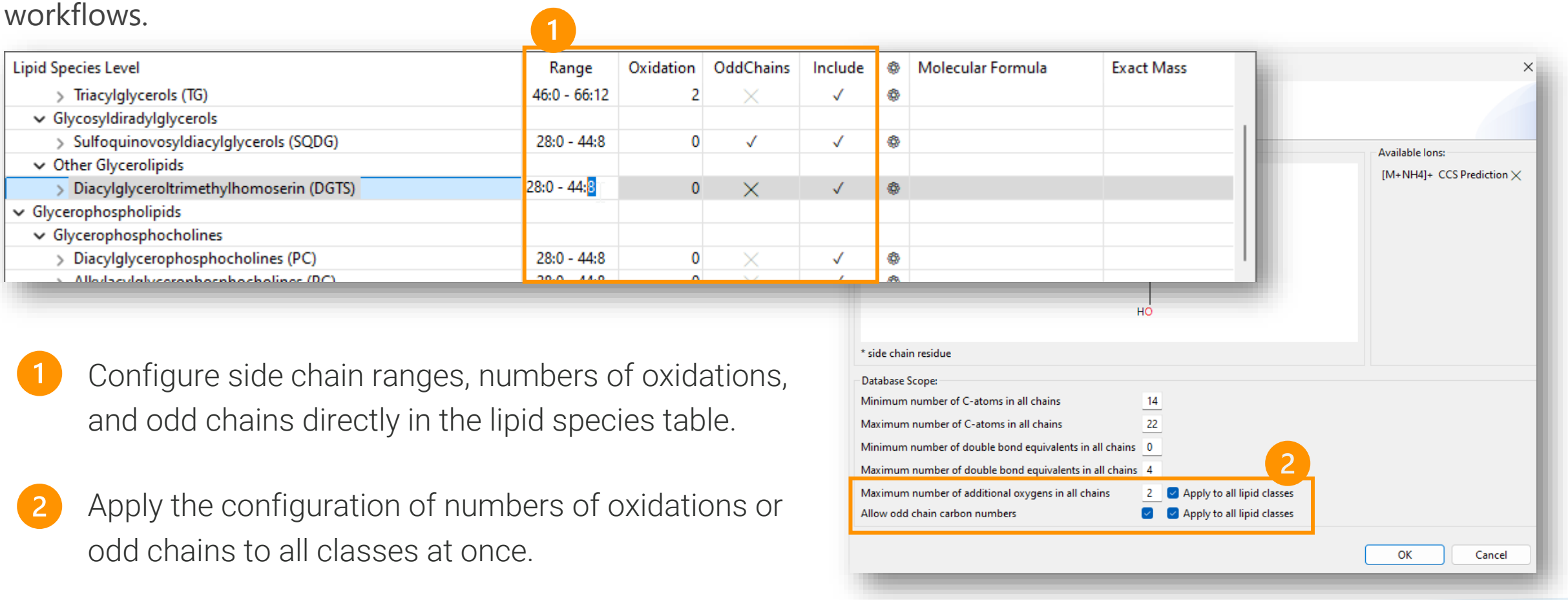
Lipid Species Annotation Extended to Include Side Chain Oxidation

The rule-based Lipid Species annotation now accounts for oxidized lipid side chains, expanding coverage and biological relevance in Lipidomics analyses.



Improved Configuration Interface for Lipid Species Annotation

Enhanced UI for defining lipid annotation rules, offering greater flexibility and transparency in lipid annotation workflows.

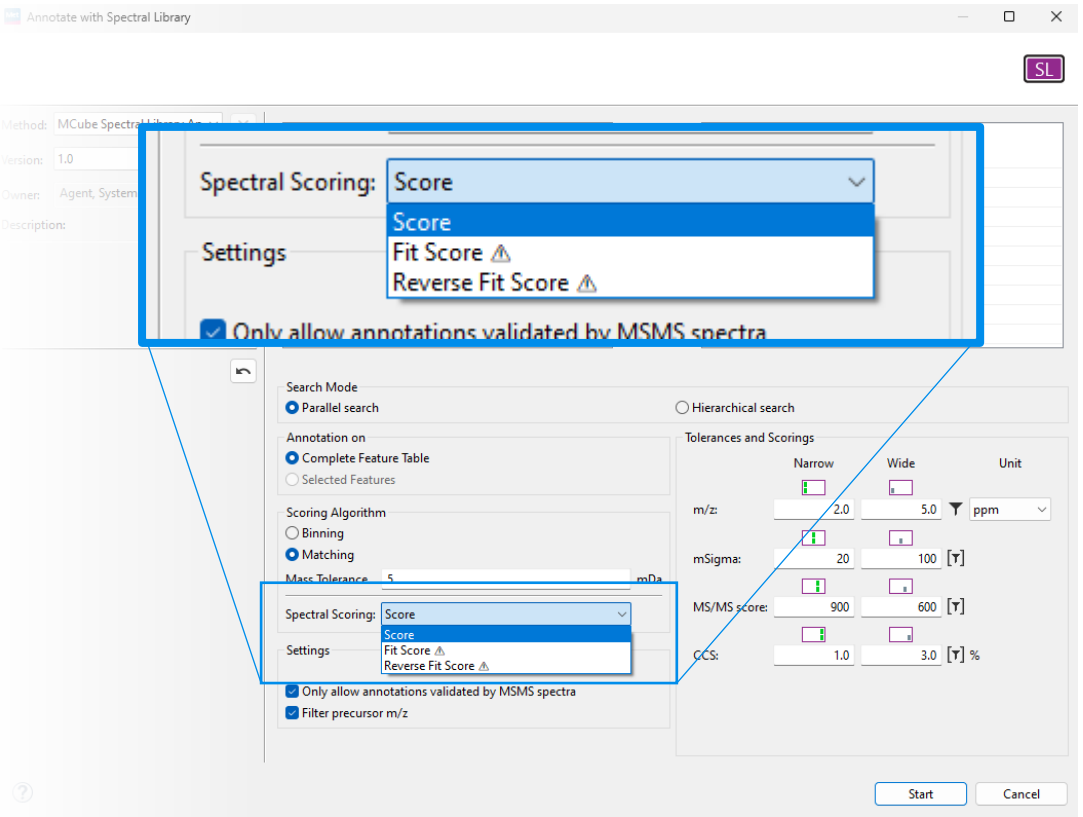


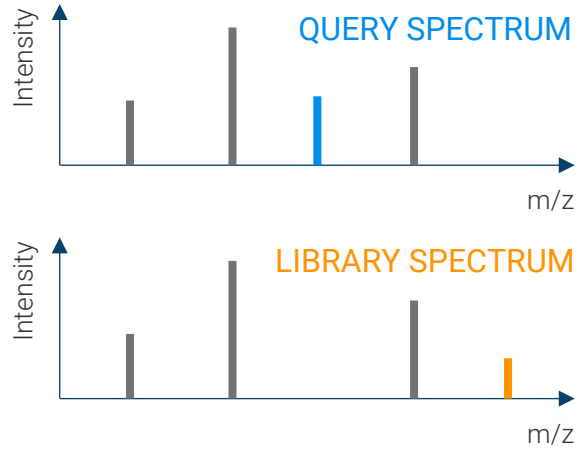
1. Configure side chain ranges, numbers of oxidations, and odd chains directly in the lipid species table.

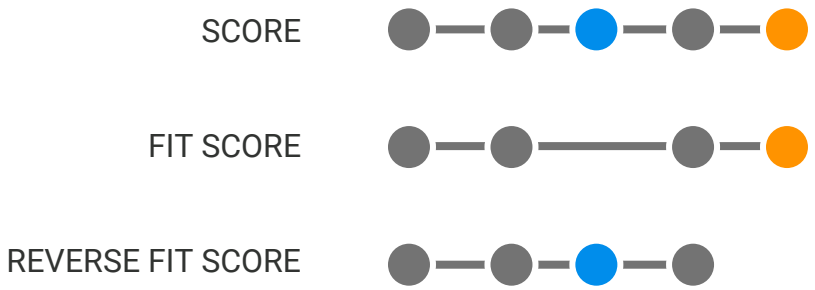
2. Apply the configuration of numbers of oxidations or odd chains to all classes at once.

Fit Score and Reverse Fit Score Added for Spectral Library Matching

New scoring metrics provide improved confidence assessment in spectral library matches, supporting more robust compound identification.







All m/z values are considered.

Only m/z values in the library reference spectrum are considered. Additional peaks in the query spectrum do not affect the score.

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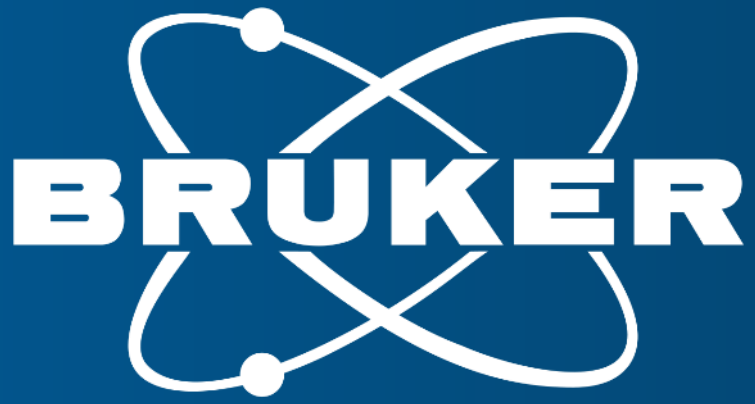

Innovation with Integrity