

# 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**
- 02 New **T-ReX<sup>2</sup>** and **T-ReX<sup>3</sup>** Workflows for **MALDI Spot** Analysis
- 03 New **T-ReX Pi3** Workflow for **DART** Processing with External Calibration
- 04 MALDI-Imaging Data Processing Transitioned to [SCiLS™ Lab](#)

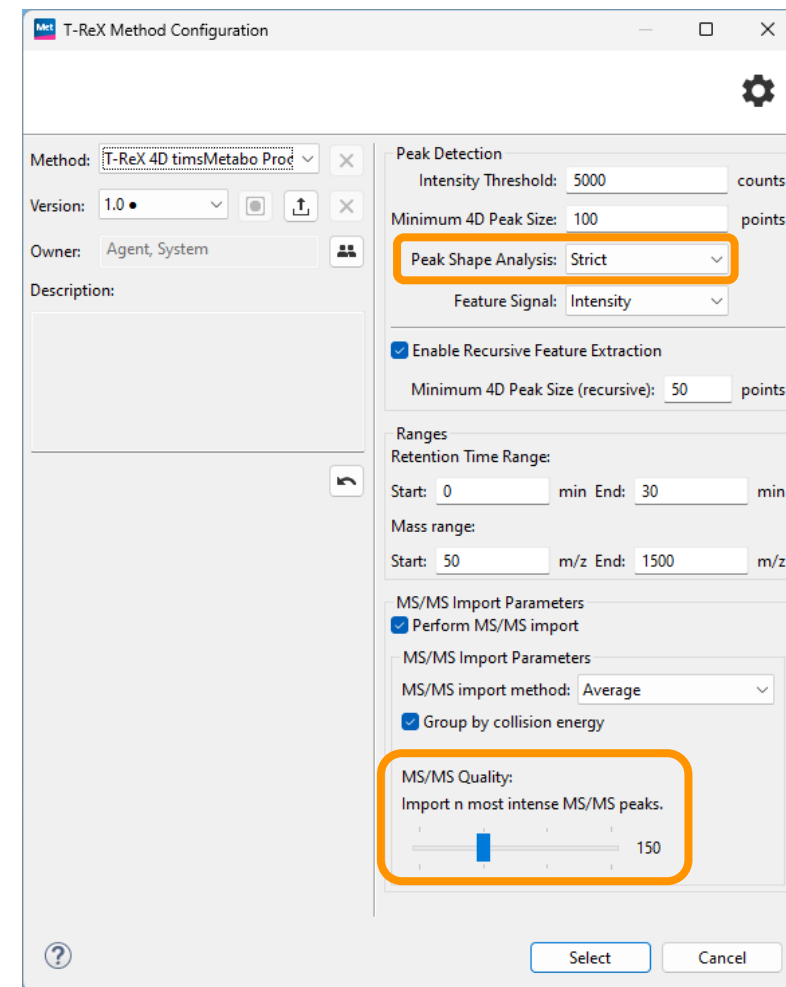
- 05 Remote Raw Data Processing via Networked Node
- 06 Refined User Interface for Sample and Analysis Setup
- 07 Lipid Species Annotation Extended to Include Side Chain Oxidation
- 08 Improved Configuration Interface for Lipid Species Annotation
- 09 Fit Score and Reverse Fit Score Added for Spectral Library Matching

## Enhanced T-ReX 4D Algorithms for timsMetabo



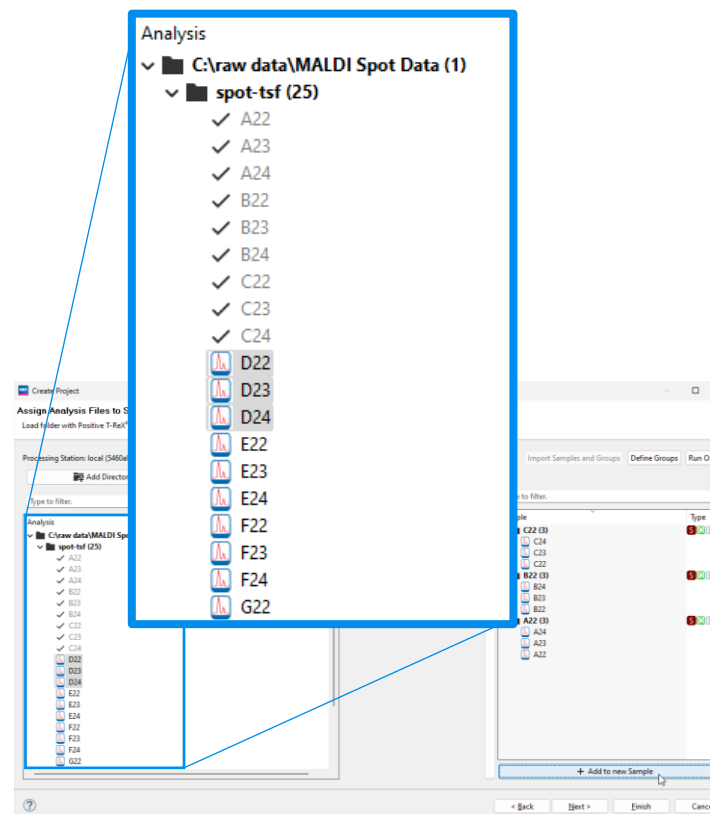
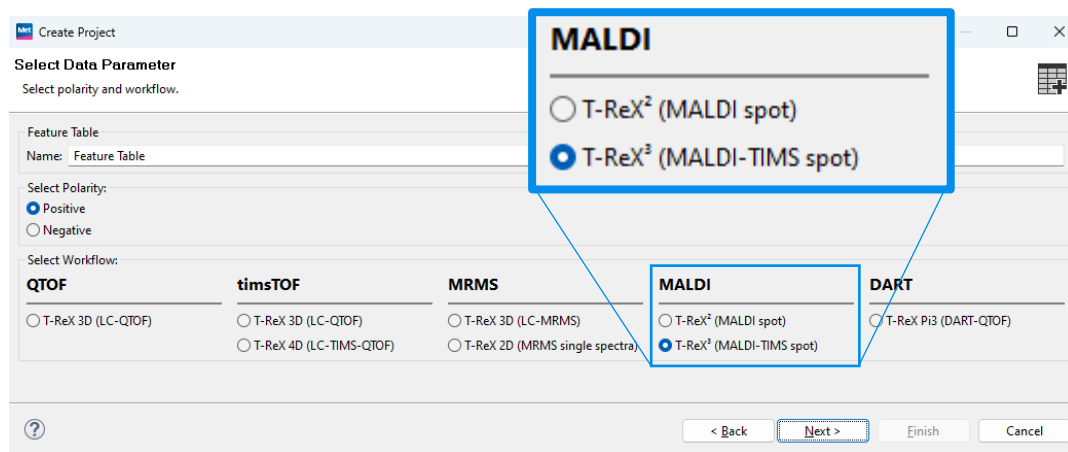
MetaboScape 2026 introduces new default processing methods for LC-TIMS-MoRE data from [timsMetabo](#).

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-ReX<sup>2</sup> and T-ReX<sup>3</sup> 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.



Mark Samples and their Analyses as Calibrants.

Folder	File	Icons
Mass Calibration_1_1 (3)	Mass Calibration_1_1_3409.d	S Q B C
	Mass Calibration_1_1_3421.d	S Q B C
	Mass Calibration_1_1_3433.d	S Q B C

Folder	File	Icons
Sample1_3_1 (3)	Sample1_3_1_3411.d	S Q B C
	Sample1_3_1_3423.d	S Q B C
	Sample1_3_1_3435.d	S Q B C
Sample2_4_1 (3)	Sample2_4_1_3412.d	S Q B C
	Sample2_4_1_3424.d	S Q B C
	Sample2_4_1_3436.d	S Q B C
Sample3_5_1 (3)	Sample3_5_1_3413.d	S Q B C
	Sample3_5_1_3425.d	S Q B C
	Sample3_5_1_3437.d	S Q B C
Sample4_6_1 (3)	Sample4_6_1_3414.d	S Q B C
	Sample4_6_1_3426.d	S Q B C
	Sample4_6_1_3438.d	S Q B C

Create Project

Sample	Calibrant
Sample9_11_1	
Sample9_11_1_3419	Mass Calibration_1_1_3409.d
Sample9_11_1_3431	Mass Calibration_1_1_3421.d
Sample9_11_1_3443	Mass Calibration_1_1_3433.d
Sample4_6_1	
Sample4_6_1_3414	Mass Calibration_1_1_3409.d
Sample4_6_1_3426	Mass Calibration_1_1_3421.d
Sample4_6_1_3438	Mass Calibration_1_1_3433.d

Sample	Calibrant
Sample9_11_1	
Sample9_11_1_3419	Mass Calibration_1_1_3409.d
Sample9_11_1_3431	Mass Calibration_1_1_3421.d
Sample9_11_1_3443	Mass Calibration_1_1_3433.d

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

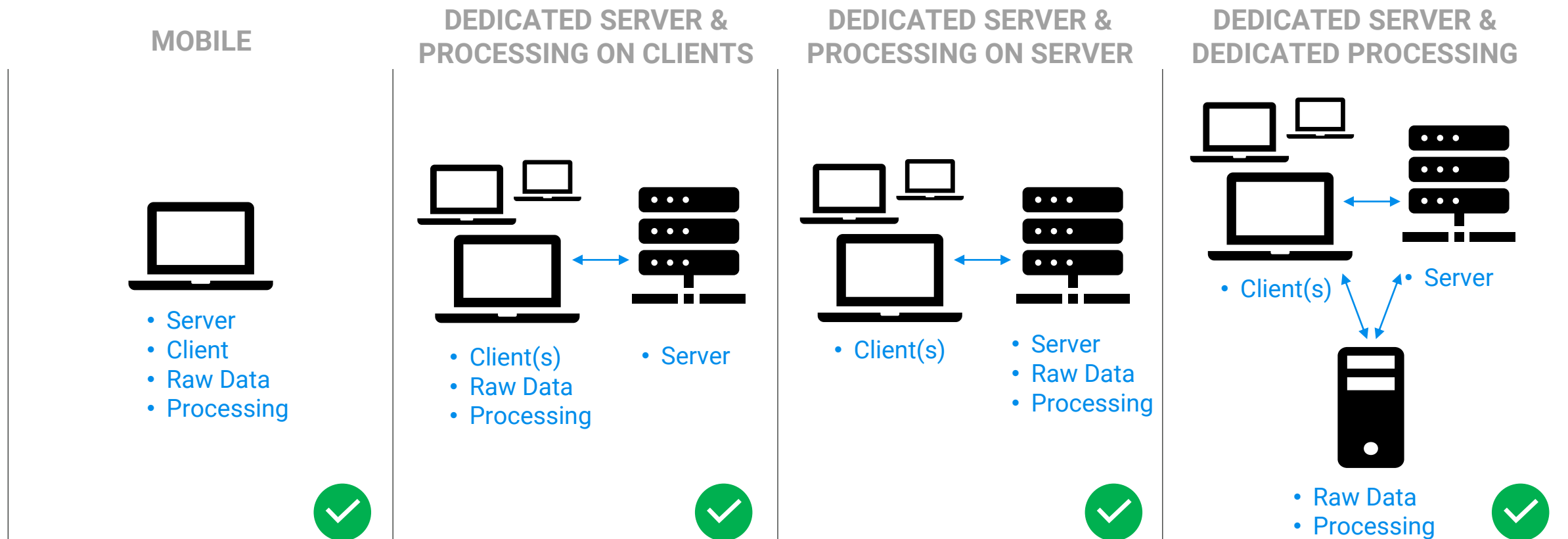
Transition of Imaging data processing from MetaboScape to SCiLS Lab is finalized. Imaging data processing in MetaboScape is obsolete.



[Click here for a video tutorial on Molecular Annotation in SCiLS Lab with MetaboScape.](#)

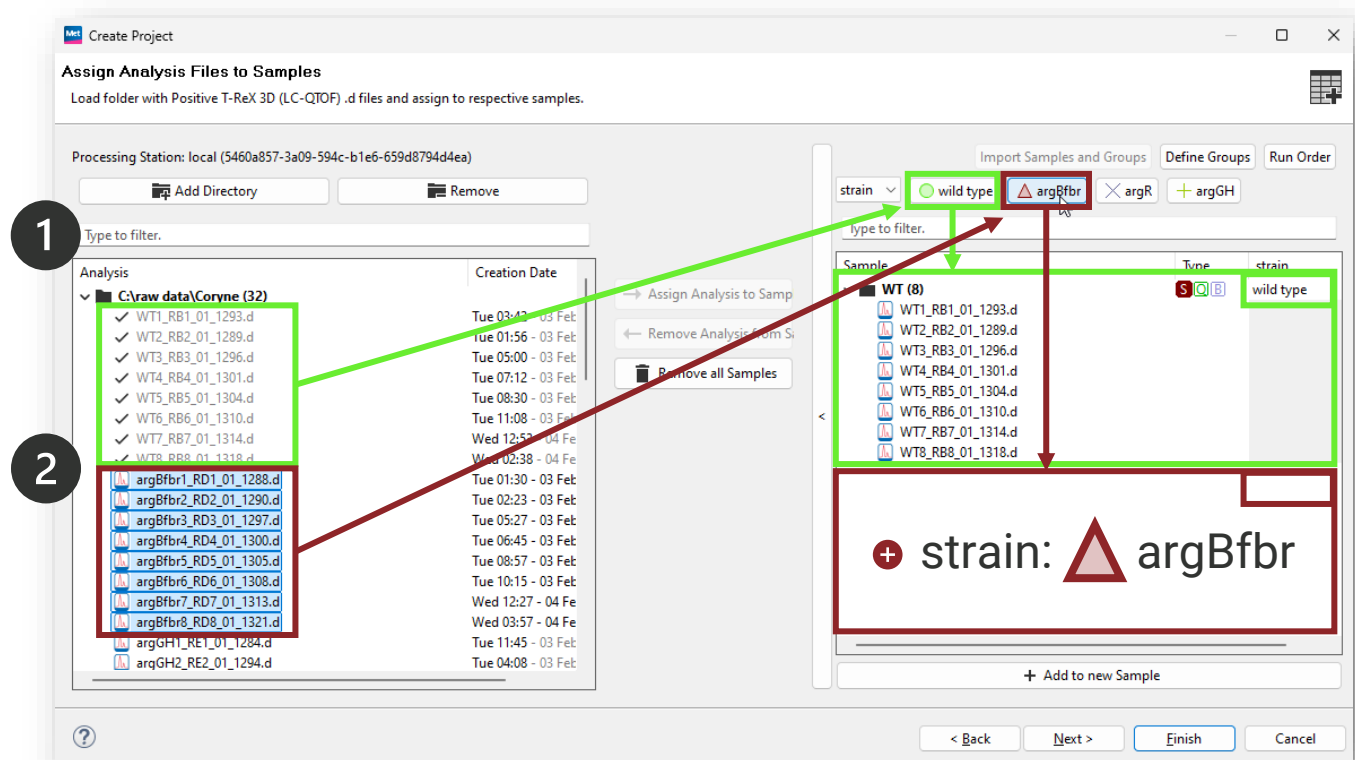
# Remote Raw Data Processing via Networked Node

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



# 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.



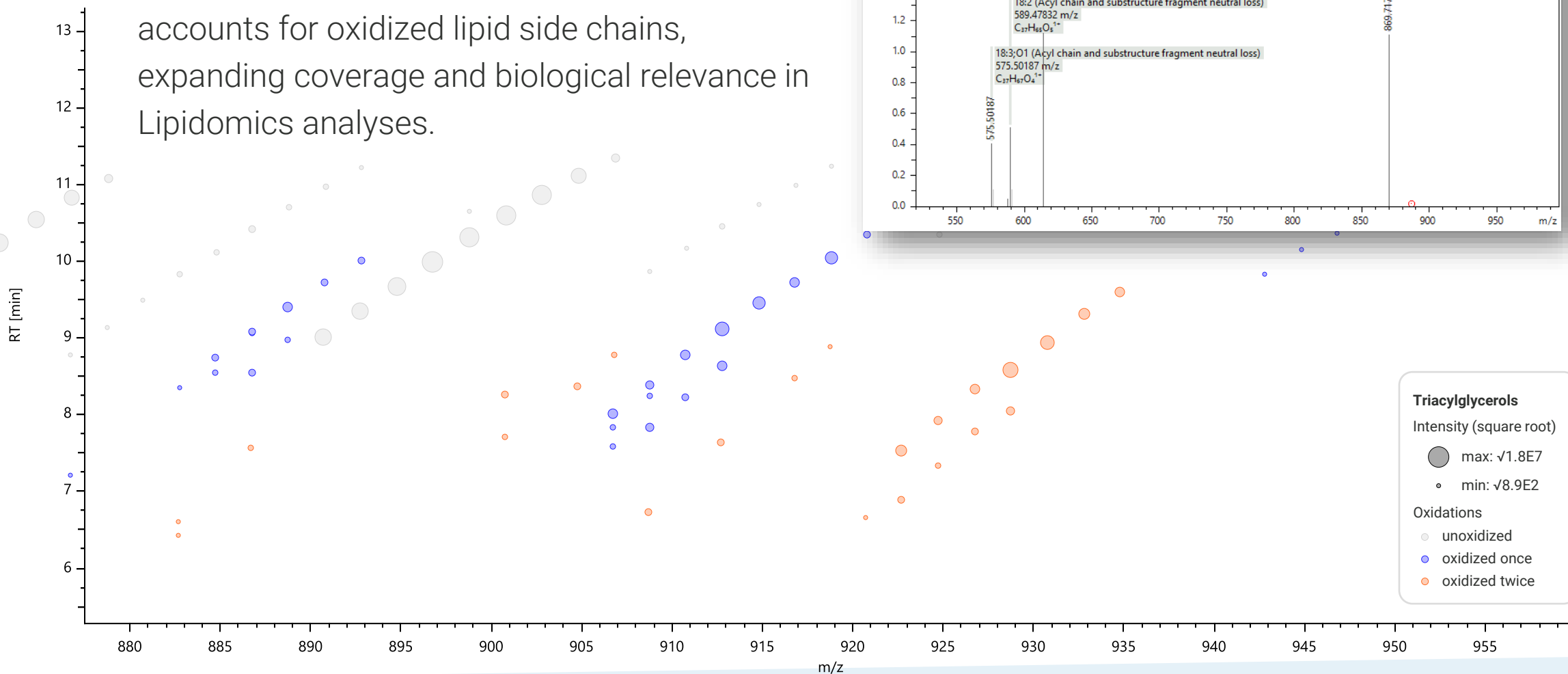
The screenshot shows the 'Create Project' window with the 'Assign Analysis Files to Samples' step. The interface is annotated with two numbered callouts:

- 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.

The 'Analysis' list on the left shows files like WT1\_RB1\_01\_1293.d and argBfbr1\_RD1\_01\_1288.d. The 'Sample' list on the right shows WT (8) samples. The 'strain' filter is set to 'wild type', and the 'argBfbr' attribute is selected. A red box highlights the 'strain: argBfbr' attribute in the sample configuration area.

# 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.

Lipid Species Level	Range	Oxidation	OddChains	Include	Molecular Formula	Exact Mass
> Triacylglycerols (TG)	46:0 - 66:12	2	✗	✓		
▼ Glycosylidirdiacylglycerols						
> Sulfoquinovosyldiacylglycerols (SQDG)	28:0 - 44:8	0	✓	✓		
▼ Other Glycerolipids						
> Diacylglyceroltrimethylhomoserin (DGTS)	28:0 - 44:8	0	✗	✓		
▼ Glycerophospholipids						
▼ Glycerophosphocholines						
> Diacylglycerophosphocholines (PC)	28:0 - 44:8	0	✗	✓		
> Alkylacylglycerophosphocholines (APC)	28:0 - 44:8	0	✗	✓		

\* side chain residue

Database Scope:

Minimum number of C-atoms in all chains

Maximum number of C-atoms in all chains

Minimum number of double bond equivalents in all chains

Maximum number of double bond equivalents in all chains

Maximum number of additional oxygens in all chains   Apply to all lipid classes

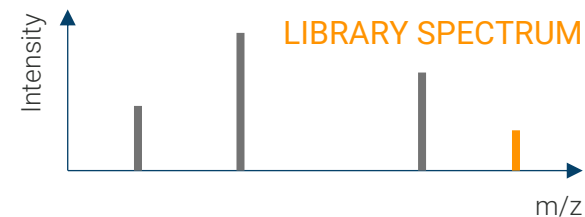
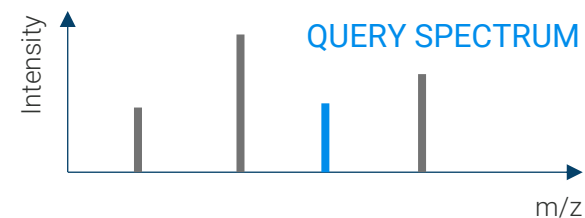
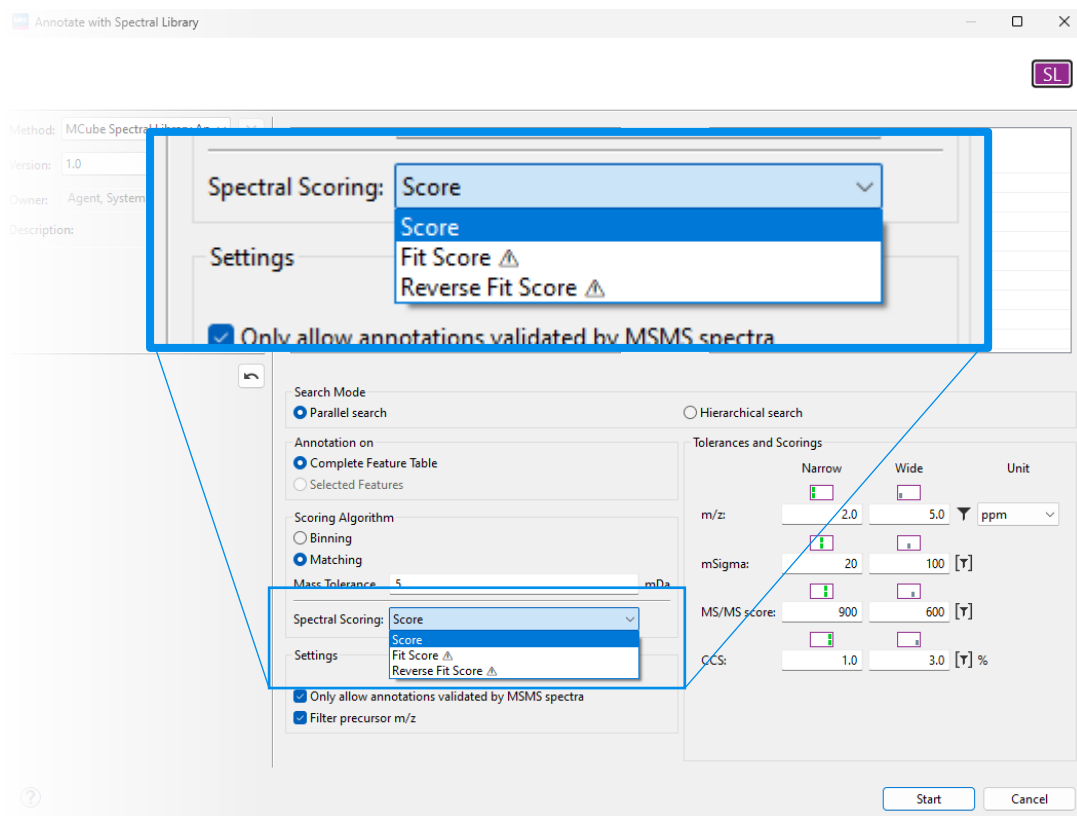
Allow odd chain carbon numbers   Apply to all lipid classes

Available Ions:  
[M+NH4]<sup>+</sup> CCS Prediction ✕

- 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.



SCORE



All m/z values are considered.

FIT SCORE

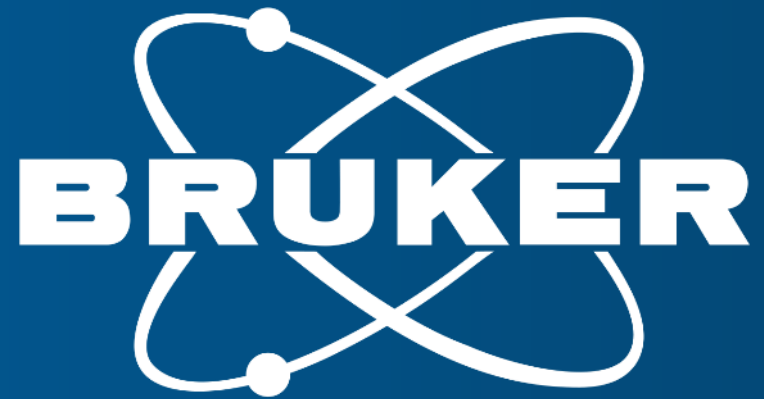


Only m/z values in the library reference spectrum are considered. Additional peaks in the query spectrum do not affect the score.

REVERSE FIT SCORE



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



Innovation with Integrity