What’s new in MetaboScape 2024b

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

Outline

01 Mixed-Mode Acquisition and Annotation

02 4D Lipidomics from PASEF to prmPASEF; Create TASQ Methods with MetaboScape

03 Context-sensitive and interactive MS/MS spectrum views

04 The BioTransformer sequence mode

05 Train SVMs on known analyses and apply to unknowns

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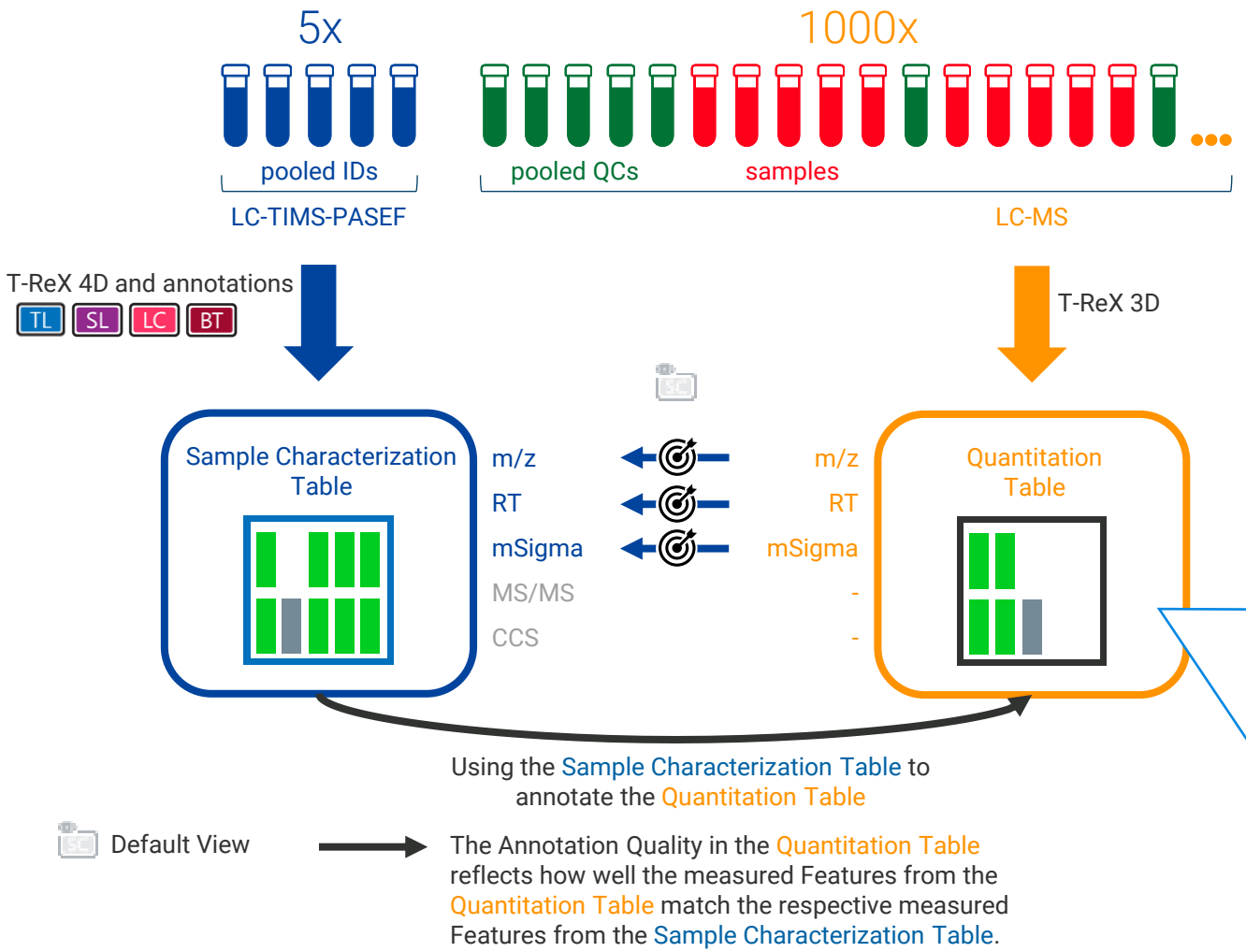
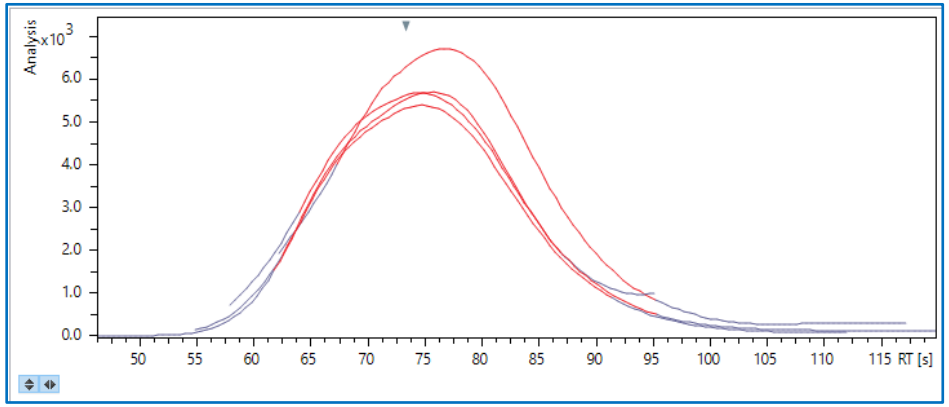
Mixed-Mode Acquisition: Annotate Features with a Characterization Table



In the Default View of the Quantitation Table, the annotations behave similarly to other annotations. The Annotation Quality indicates the alignment between the Sample Characterization Table and the Quantitation Table. Furthermore, additional information, including extracted ion chromatograms and spectra, is sourced from the Quantitation Table, as per usual.



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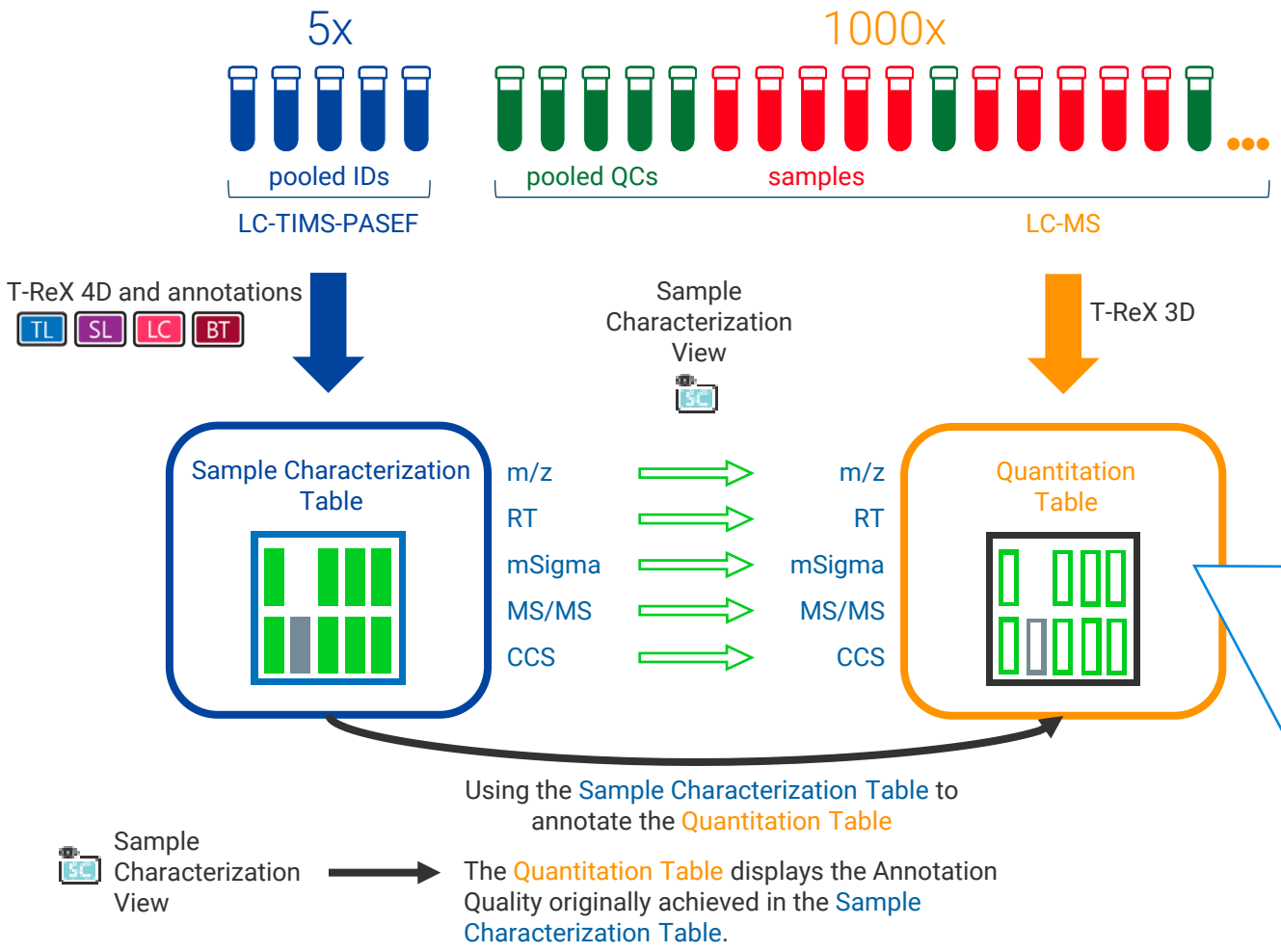
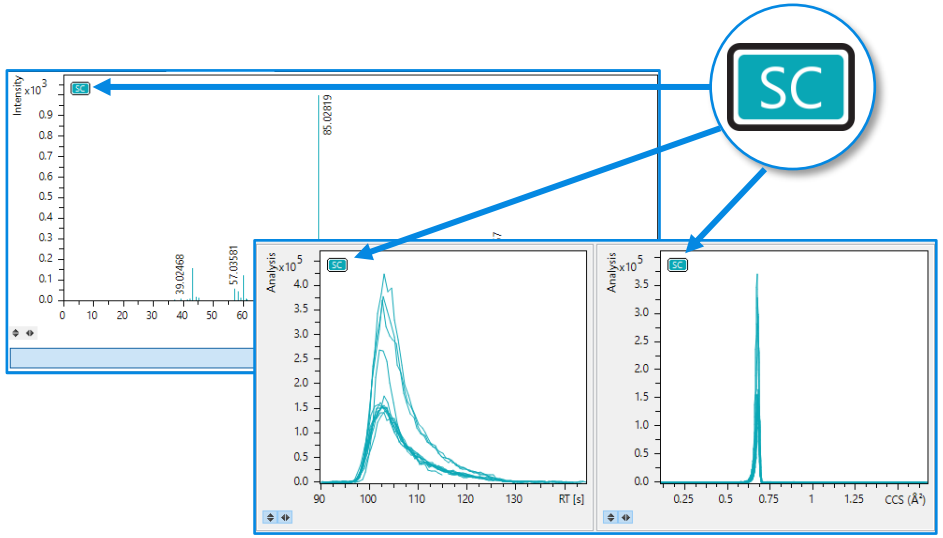
Mixed-Mode Acquisition: Review the referenced high dimensional Annotation Quality



In the Sample Characterization View, the Annotation Quality symbols for annotations in the Quantitation Table are substituted with those from the Features in the Sample Characterization Table.

If available, the EIC, EIM, and MS/MS views present data derived from the Features in the Sample Characterization Table. Turquoise icons and view borders indicate that referenced data is being displayed.



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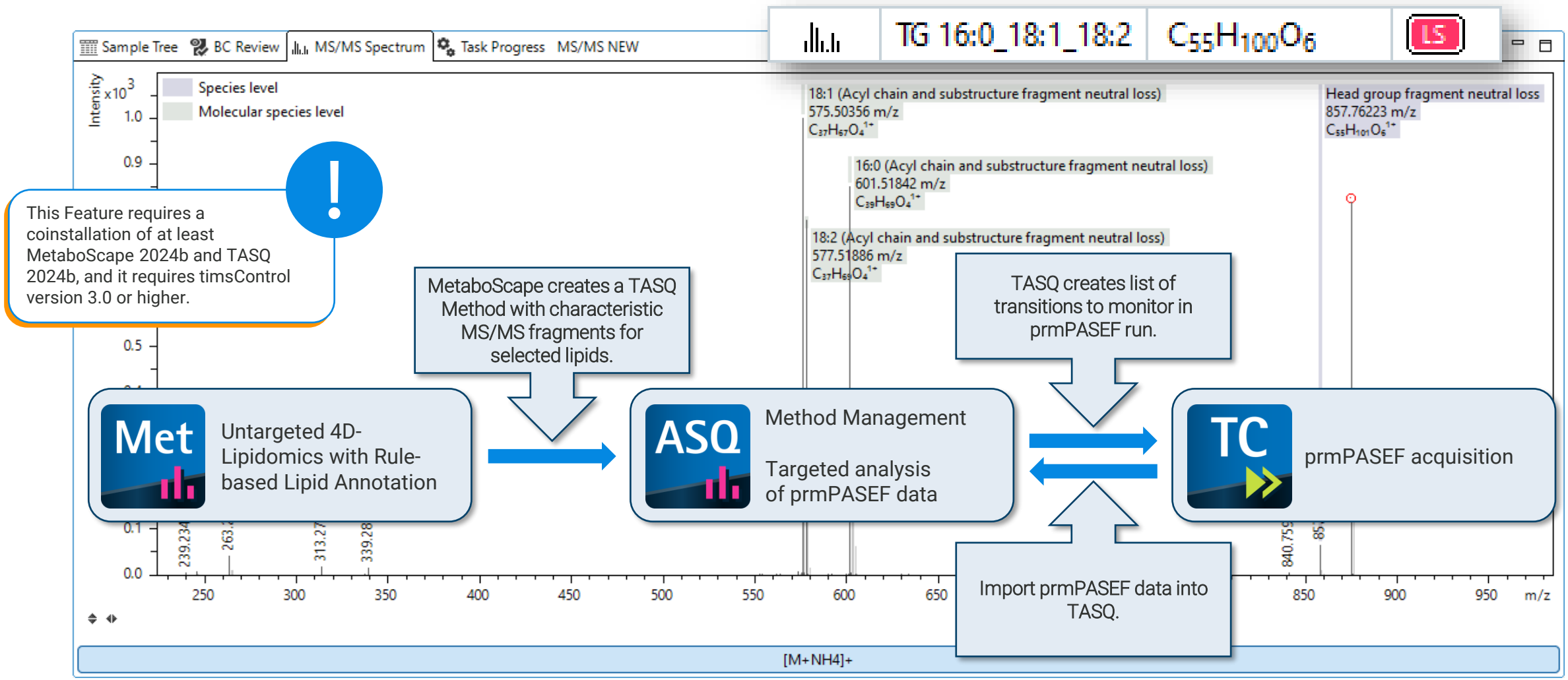
Towards targeted and quantitative 4D Lipidomics - From PASEF to prm-PASEF



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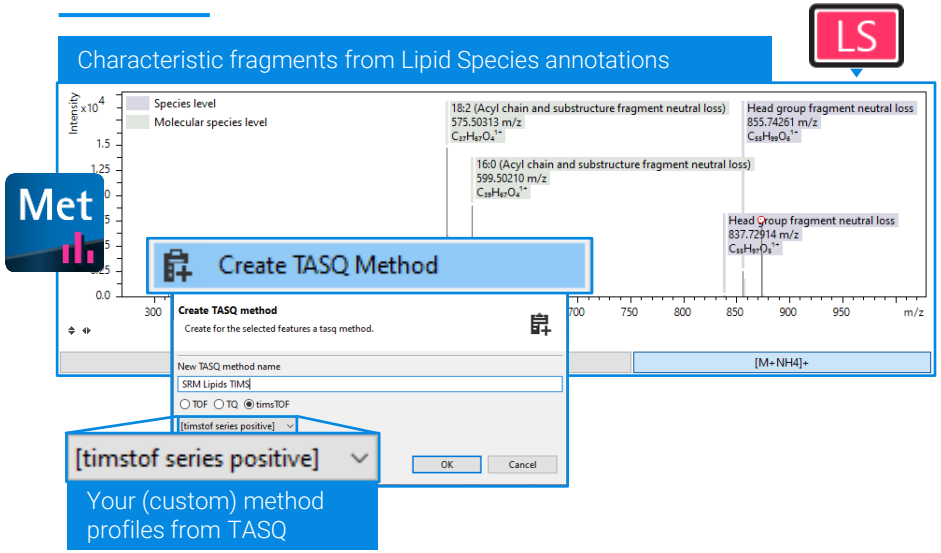
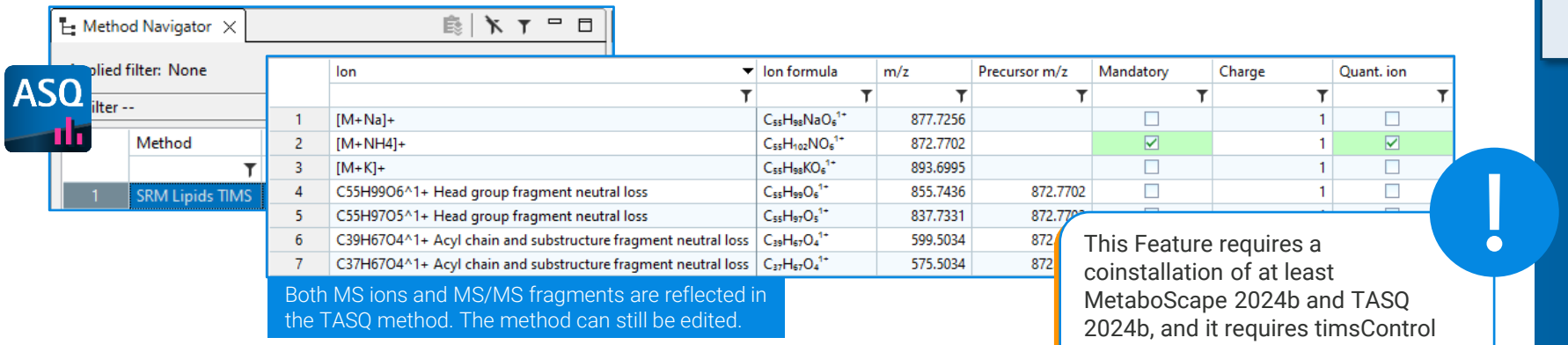
Generate TASQ methods from within MetaboScape



Select one or more features of interest from the Feature Table to incorporate them as precursors (Ion m/z, RT, and CCS) into a TASQ method. Specifically for Lipidomics, i.e., for features annotated with the rule-based lipid species annotation tool (LS), characteristic MS/MS fragments will be included.

Upon submission from MetaboScape, the new method is instantly displayed in TASQ. This method can then be further refined and optimized using TASQ's dedicated method editor, providing a seamless and efficient workflow for method creation and curation.



This Feature requires a coinstallation of at least MetaboScape 2024b and TASQ 2024b, and it requires timsControl version 3.0 or higher.

Met — Untargeted 4D-Lipidomics with Rule-based Lipid Annotation

MetaboScape creates a TASQ Method with characteristic MSMS fragments for selected lipids.

ASQ — Method Management

Targeted analysis of prmPASEF data

TASQ creates list of transitions to monitor in prmPASEF run.

Import prmPASEF data into TASQ.

TC — prmPASEF acquisition

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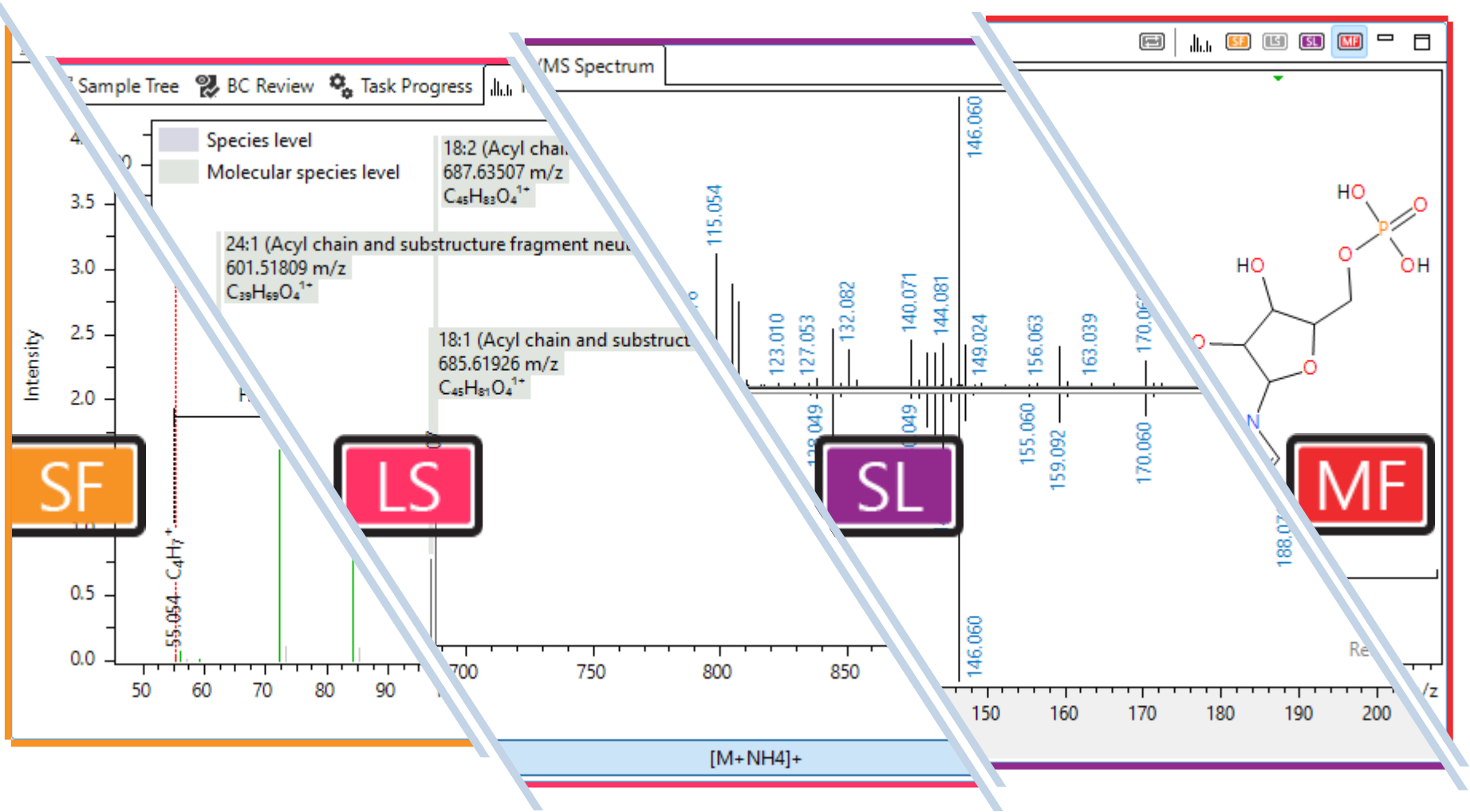
Context-sensitive and interactive MS/MS spectrum views



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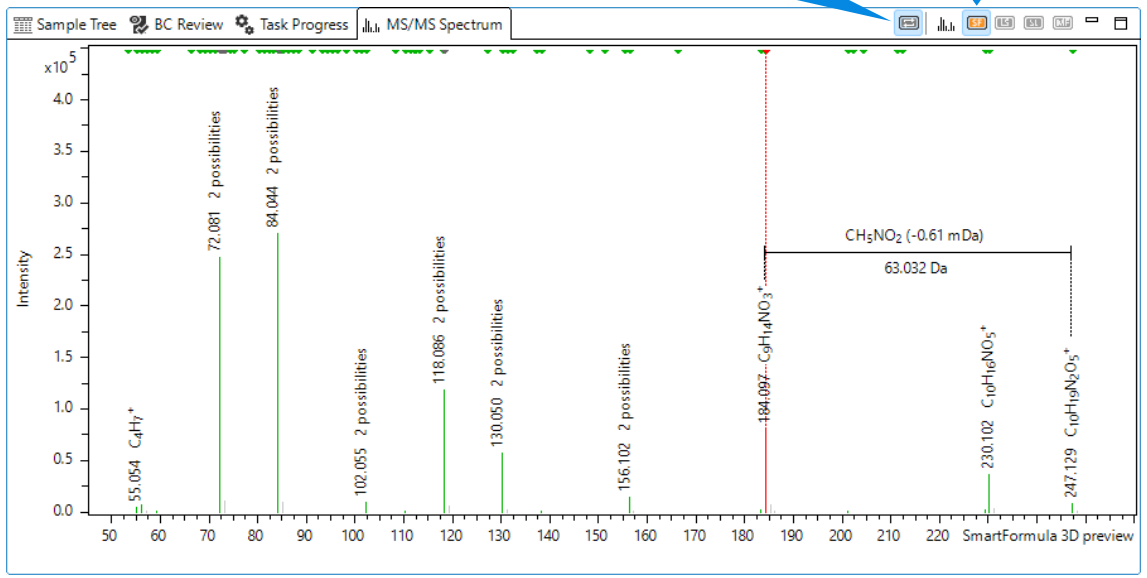
Context-sensitive and interactive MS/MS spectrum views

With the context-sensitive auto selection of the most suitable MSMS spectrum visualization, you will always have the most relevant information at your finger tips.

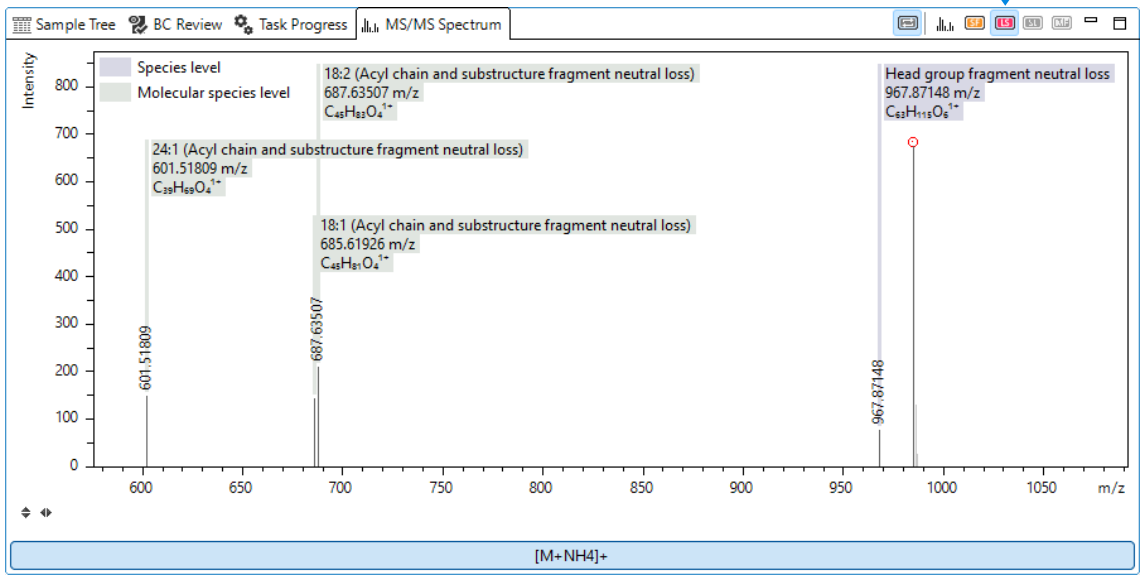
SF



This option becomes accessible when the Feature has been annotated with a molecular formula.

The Smart Formula 3D tool provides annotations for fragment peaks using plausible subformulas derived from the precursor's ion formula. By dragging a ruler from one peak label to another, you can calculate the distance between them and identify potential neutral losses that could account for this measured distance.

LS



This option is enabled when the Feature has been annotated using the rule-based Lipid Species annotation tool.

Characteristic fragment peaks are annotated with both their m/z value and ion formula. However, the most crucial aspect is the presentation of their relevance for the respective species level or molecular species level annotation. This valuable information can now be transferred to TASQ, facilitating the generation of a targeted method specifically for selected lipid species.

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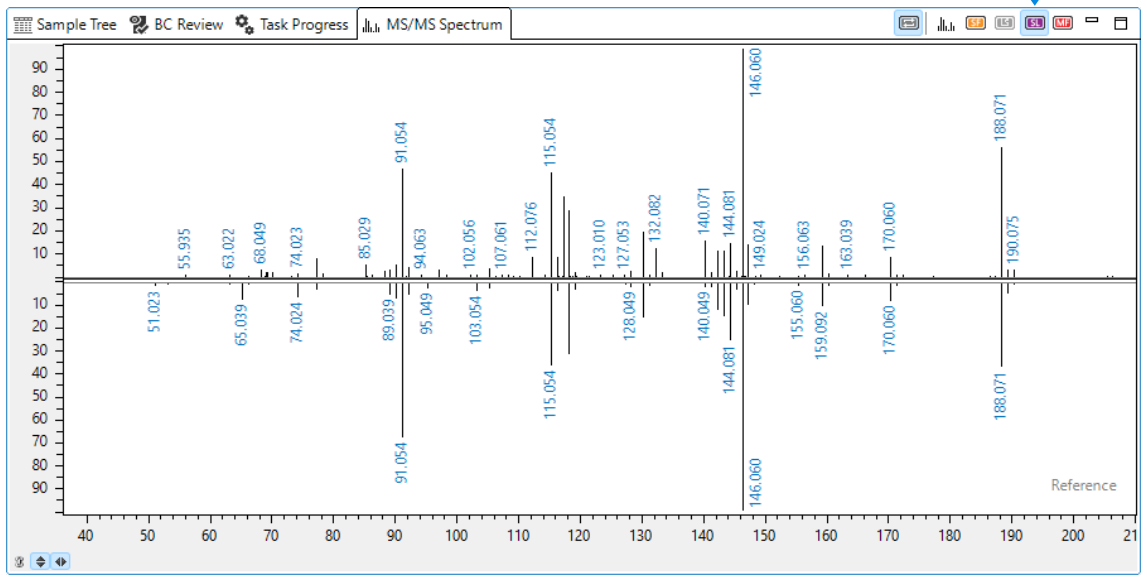
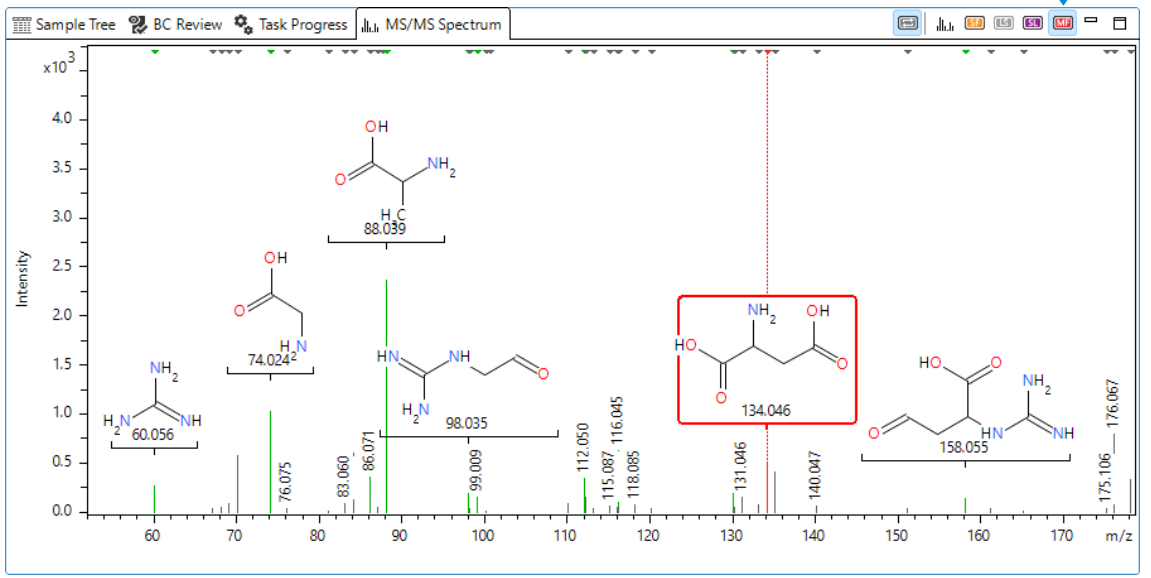
Context-sensitive and interactive MS/MS spectrum views



This option is made available once the Feature has been annotated using a Spectral Library.

The display is divided into two sections: the upper section presents the measured spectrum, while the lower section exhibits the reference spectrum derived from the Spectral Library. Despite the ability to zoom and pan across the spectra, the x-axes remain synchronized, ensuring a consistent and comparative view of the data.



This option becomes available when the Feature has been supplemented with structural information.

The MetFrag *in-silico* fragmentation process is automatically initiated, resulting in the annotation of corresponding fragments within the spectrum. By left-clicking on a fragment structure, it gets highlighted within the precursor's structure in the structure view, providing a clear visual correlation. Furthermore, right-clicking on a fragment allows you to filter the Feature Table, unveiling other Features that share the same fragment peak.

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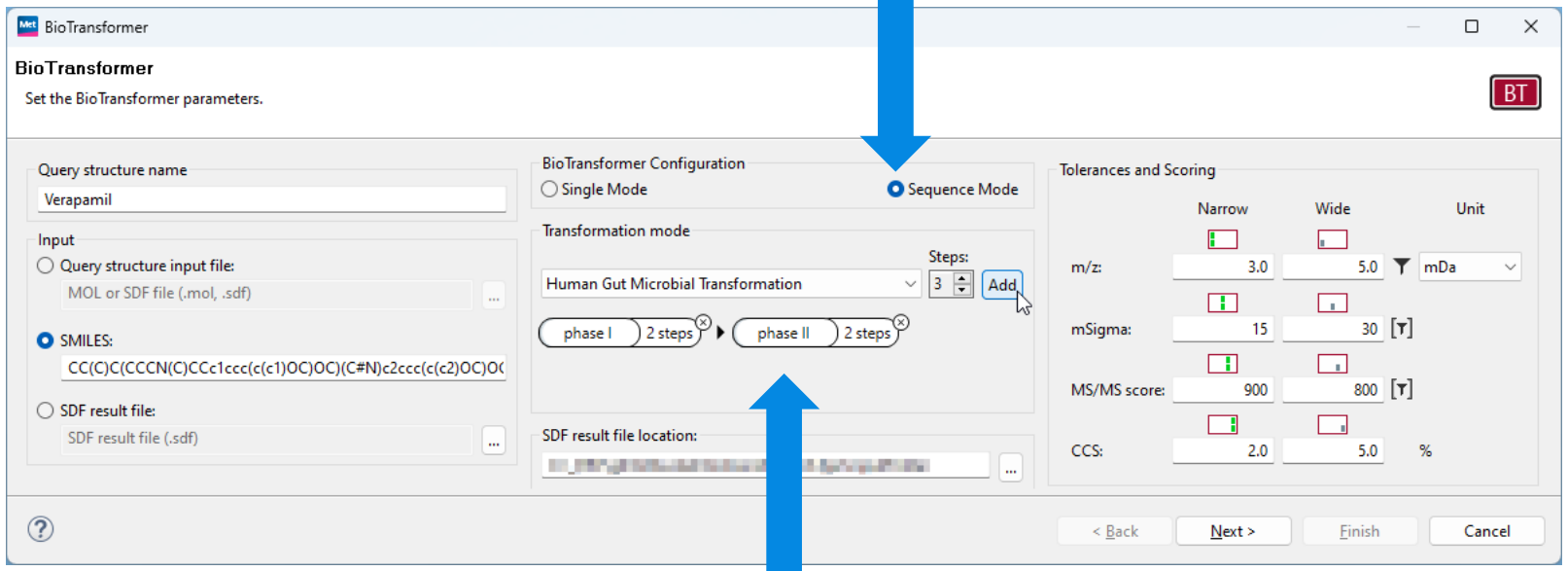
BioTransformer's sequence mode

1 Select „BioTransformer …" from the „Annotation" menu and activate the „Sequence Mode" in the „Configuration" section.



2 Build your own sequence in the „Transformation mode" section. Select the transformation model and how many steps to perform, and click the „Add" button to extend the sequence.

BioTransformer* offers the capability to execute a custom sequence of multiple transformations. With its integration into MetaboScape, users can conveniently configure these sequences directly within the user interface. A custom sequence can encompass multiple transformations, each iterated in one to three steps, offering a flexible and customizable approach to metabolic transformation.

* Djoumbou-Feunang et al.;
Journal of Cheminformatics 2019, 11:2

Wishart et al.;
Nucleic Acids Research 2022, 50:1

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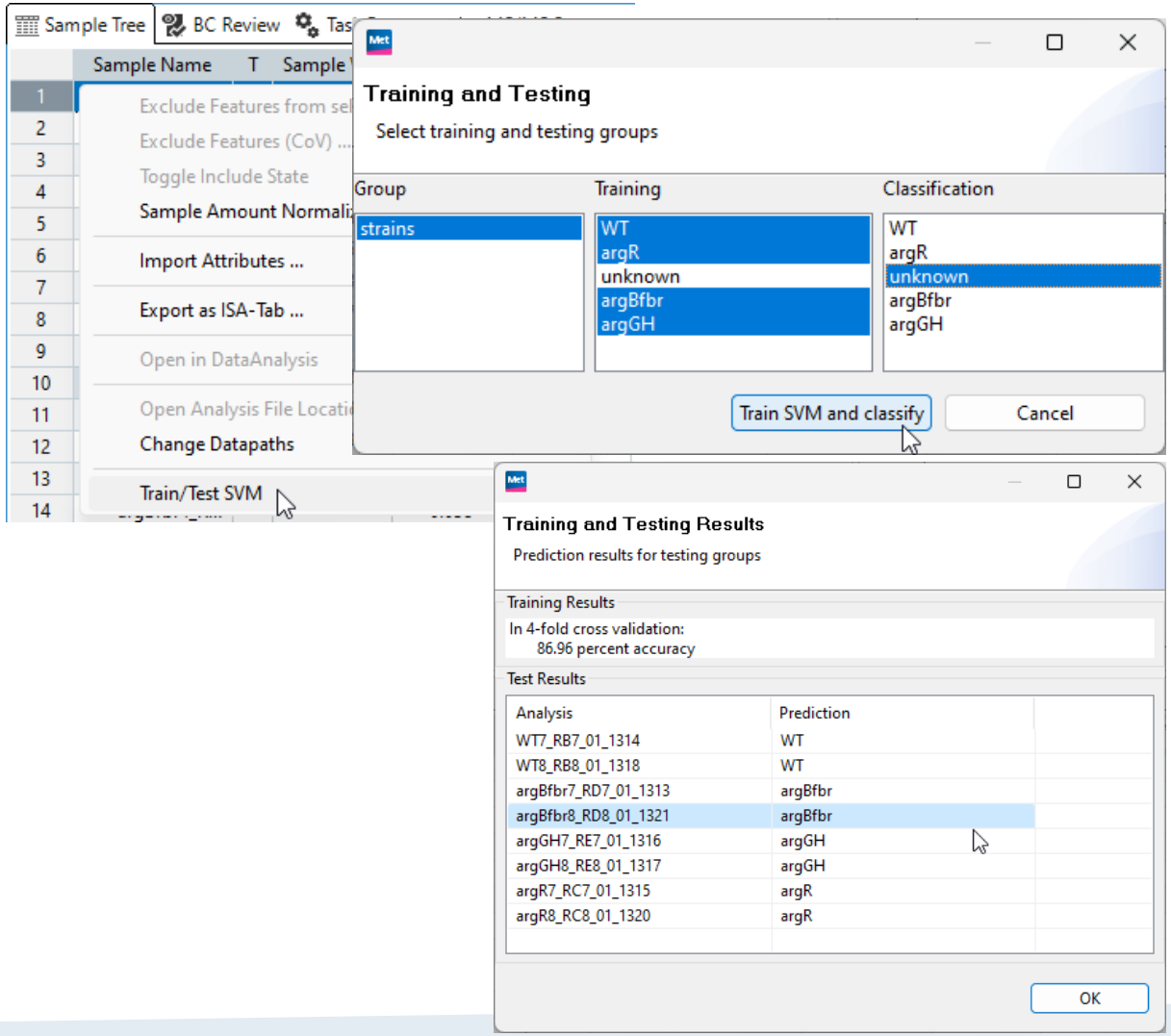
SVM Classification of unknown Samples



Begin by training a Support Vector Machine (SVM) model using replicates of known sample types. Once the model is trained, apply it to predict the sample types for unassigned analyses. To configure the experimental design, utilize the statistical groups from the Sample Tree.

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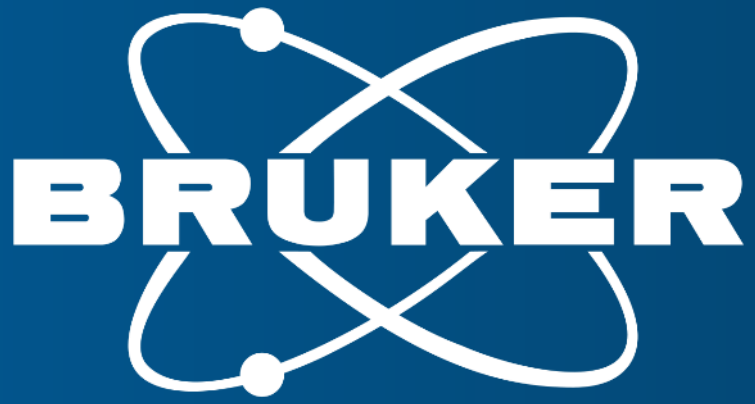

Innovation with Integrity