What’s new in MetaboScape® 2025

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

Outline

01 *in-silico* Derivatization

02 dda-PASEF to prm-PASEF

03 iprm-PASEF SpatialOMx with rule-based lipid annotation via REST API

04 Type 1 abundance error correction

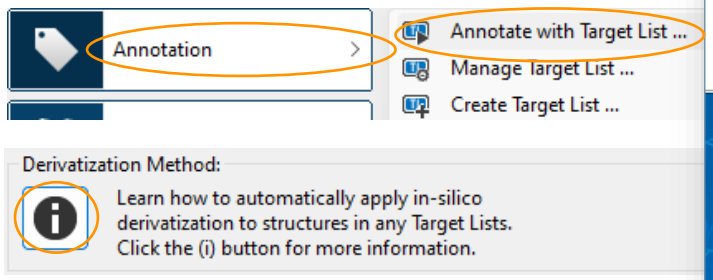
05 SVM classification as statistical view

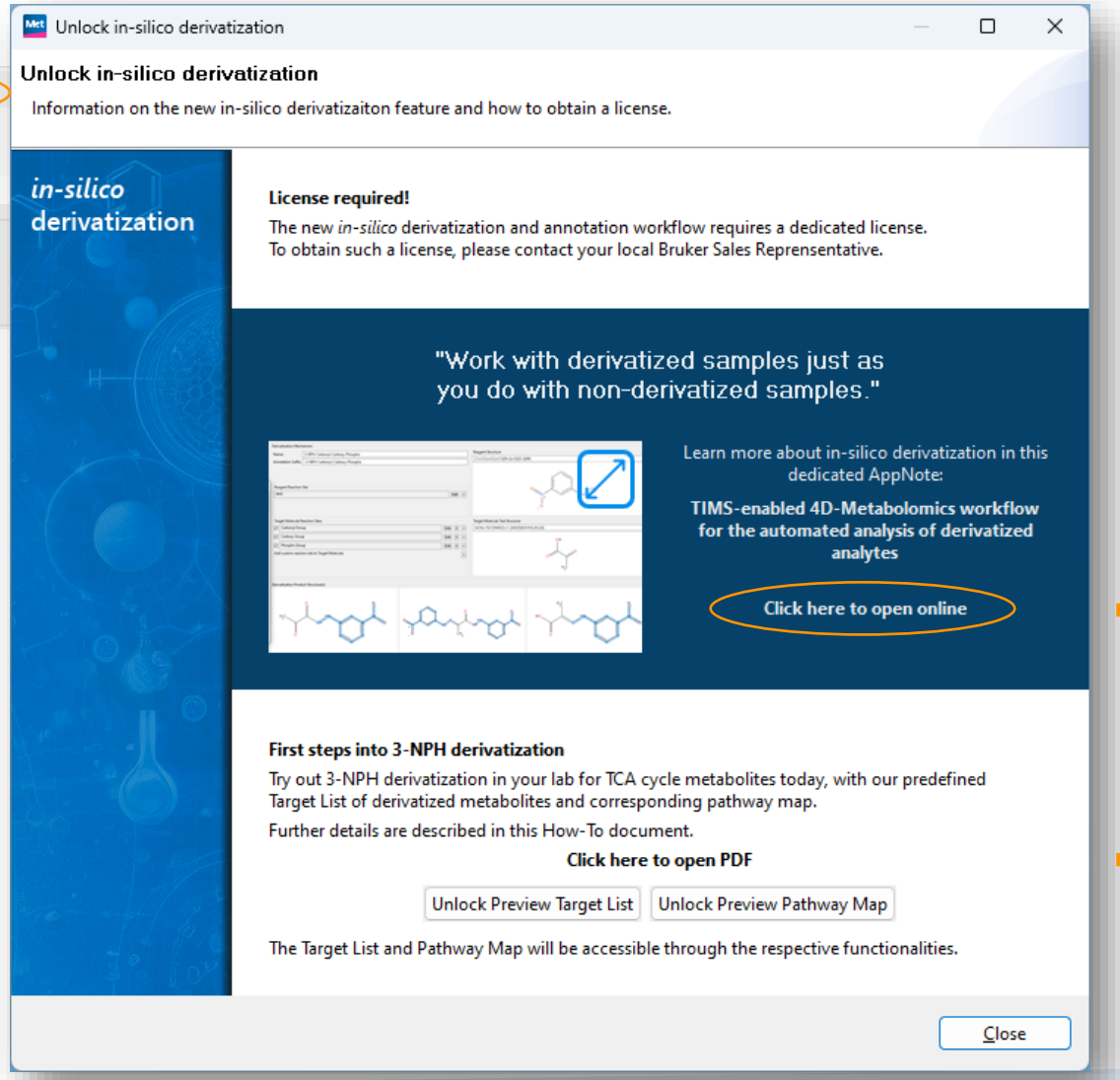
06 Export images from KMD (Survey) plot

07 Volcano plot colors according to statistical groups

in-silico derivatization with MetaboScape

Learn more about the new workflow in MetaboScape





The new *in-silico* derivatization feature is fully integrated with Target List annotation, but it requires a dedicated software license.

If the software license cannot be detected, the information shown on this slide will be presented instead.

To obtain such a license, please contact your local Bruker Sales Representative.

➡ Open AppNote on bruker.com

➡ The HowTo document, a prepared Target List with already derivatized TCA metabolites and the respective Pathway Map are installed with the MetaboScape 2025.

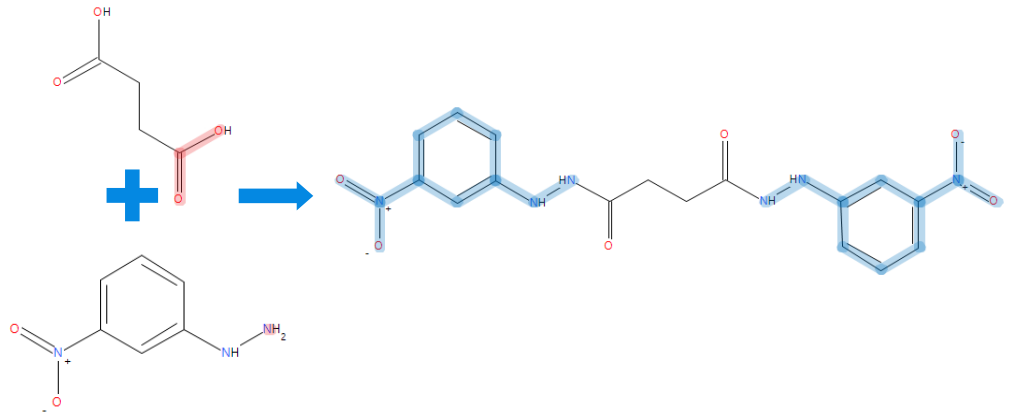
in-silico derivatization with MetaboScape

TIMS-enabled 4D-Metabolomics workflow for the automated analysis of derivatized analytes

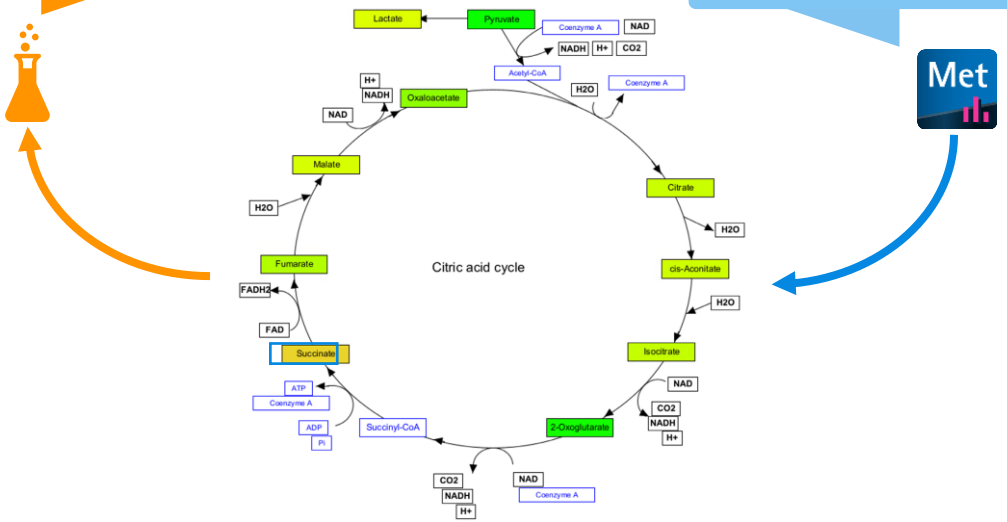
This Feature requires a dedicated software license.

BRUKER

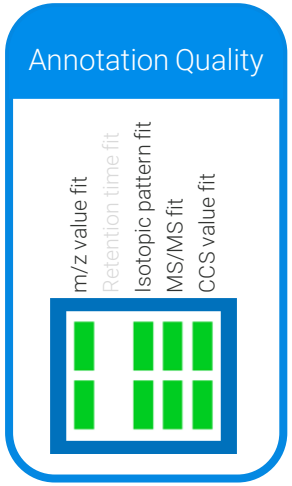
Derivatization



in-silico Derivatization



- CCS-Predict Pro
- MetFrag *in-silico* fragmentation
- True isotopic pattern

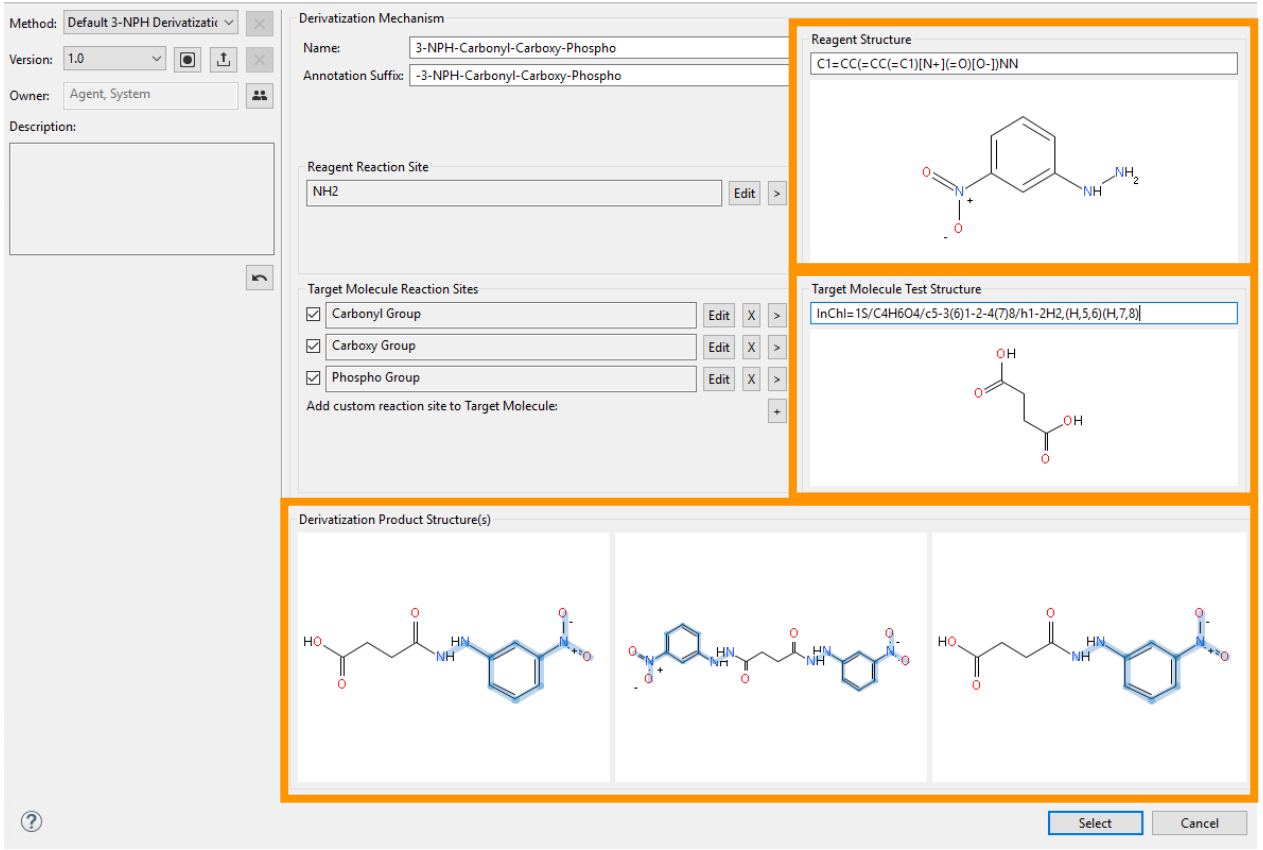


Starting from a known compound, e.g. from citric cycle, the derivatized structure, it's CCS value, and it's MSMS fragmentation are generated *in-silico* in MetaboScape.

Work with derivatized samples just as you do with non-derivatized samples

MetaboScape allows to easily tailor *in-silico* derivatization parameters for custom derivatization settings by….

This Feature requires a dedicated software license.



1

Your Choice!

Configure your derivatization reagent and how it reacts with functional groups.
Default method provided!

2

Works fully automated with your Target List annotation

All structures in the Target List are subjected to *in-silico* derivatization.

3

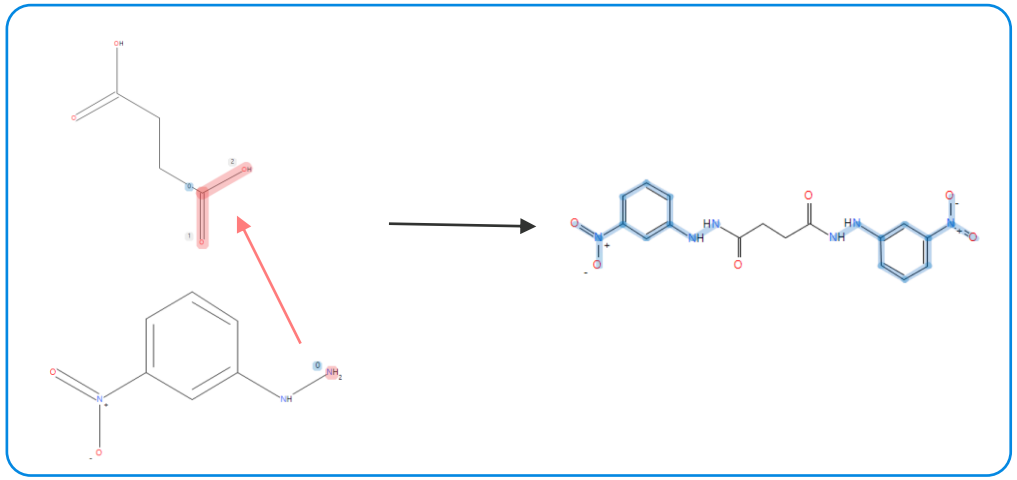
All derivatization products generated *in-silico*

All combinations of derivatization sites are computed and matched against the Feature Table.

Validate *in-silico* generated derivatization products with CCS-Predict Pro and MetFrag fragmentation

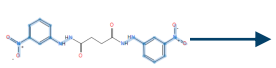
This Feature requires a dedicated software license.

4 Detected Features in the Feature Table are matched against the compounds in the Target List and their derivatives.



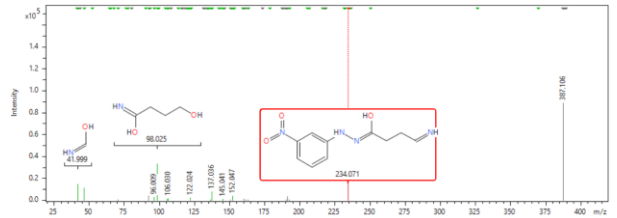
Starting from a known compound, e.g. from citric cycle, the derivatized structure, it's CCS value, and it's MSMS fragmentation are generated *in-silico* in MetaboScape.

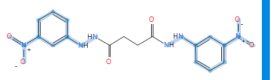
CCS-Predict Pro



Mob. 1/K0	CCS (Å²)	ΔCCS [%]	Name
0.955	198.1	1.8	Succinic acid_2-3-NPH-Ca...

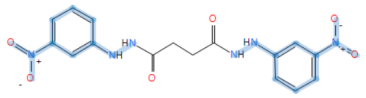
MetFrag *in-silico* fragmentation

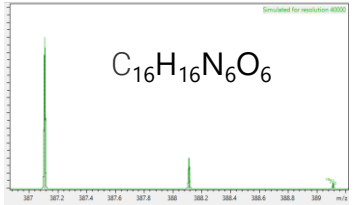




Wolf, S. *et al.*, 2010

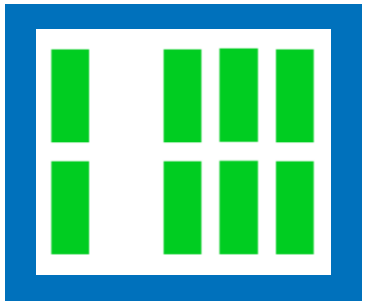
True isotopic pattern



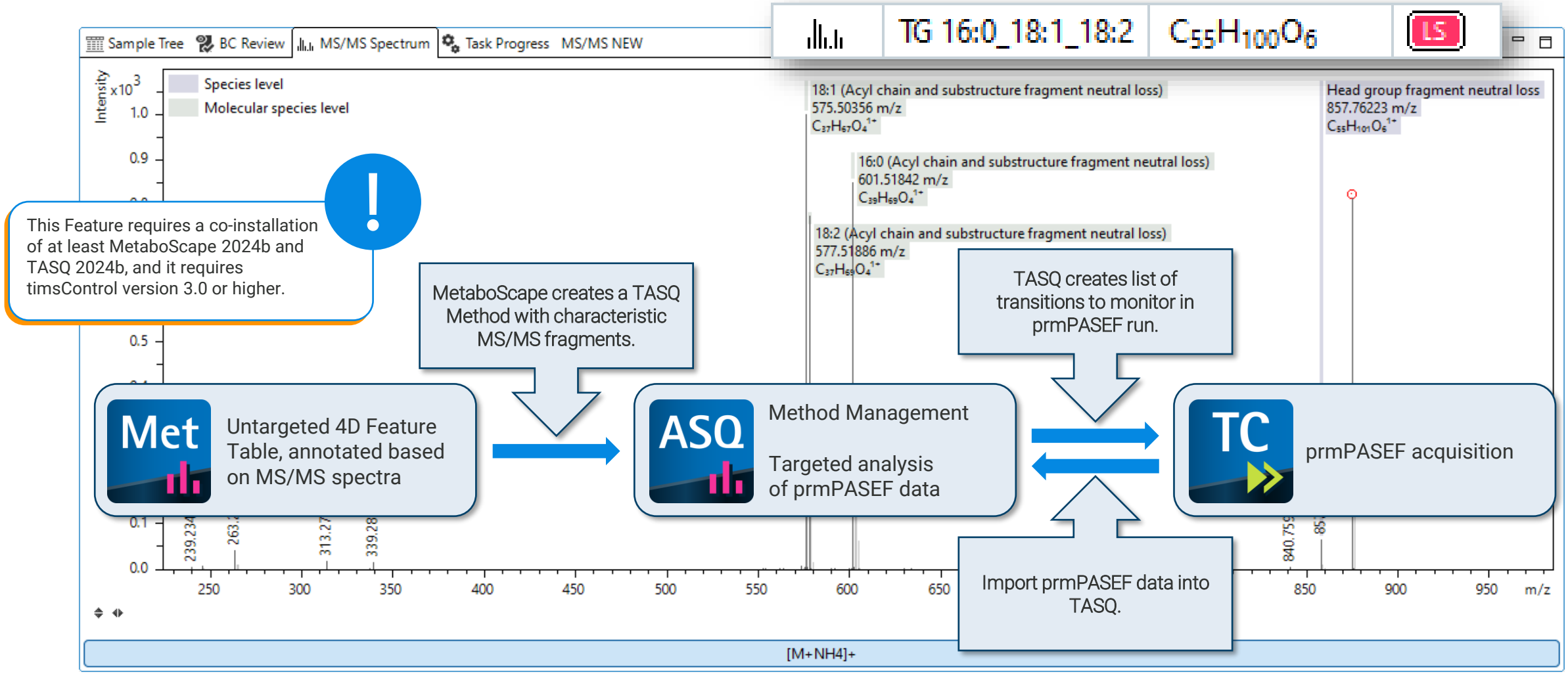


Annotation Quality

m/z value fit
Retention time fit
Isotopic pattern fit
MS/MS fit
CCS value fit



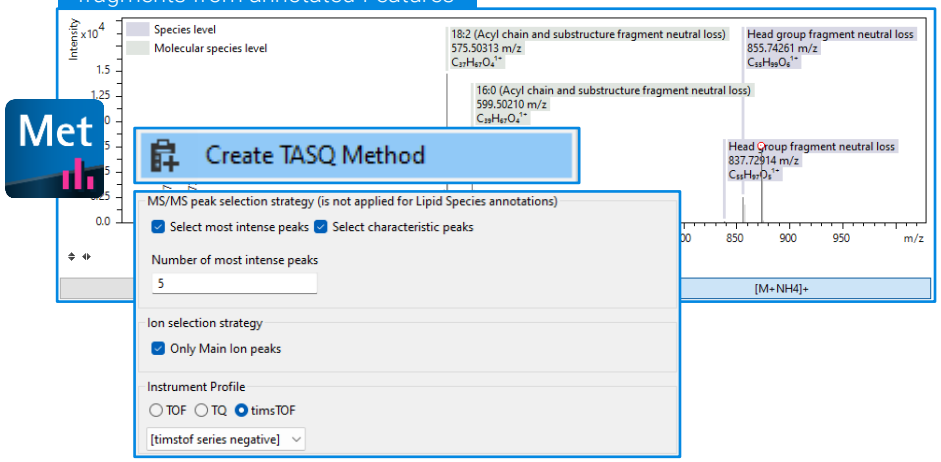
Towards targeted and quantitative 4D Lipidomics or 4D Metabolomics From PASEF® to prm-PASEF®



Generate TASQ methods from within MetaboScape

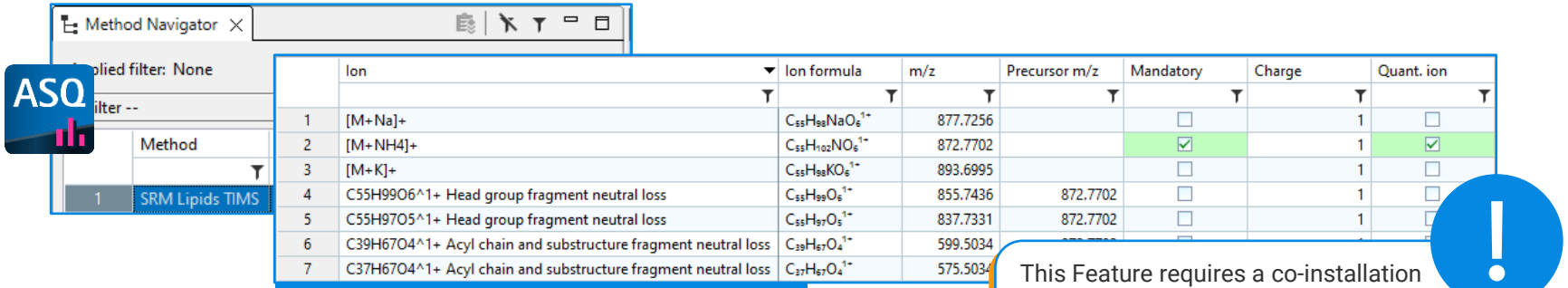
Characteristic and/or abundant fragments from annotated Features

LS | TL SL MF ...



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 tool, characteristic MS/MS fragments will be included. For all other types of annotations, the most abundant MS/MS fragments and/or characteristic MS/MS fragments (unique in their retention time range) are 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.



Both MS ions and MS/MS fragments are reflected in the TASQ method. The method can still be edited.

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

Met — Untargeted 4D Feature Table, annotated based on MS/MS spectra

MetaboScape creates a TASQ Method with characteristic MS/MS fragments.

ASQ — Method Management

Targeted analysis of prmPASEF data

TASQ creates list of transitions to monitor in prmPASEF run.

Import prmPASEF data into TASQ.

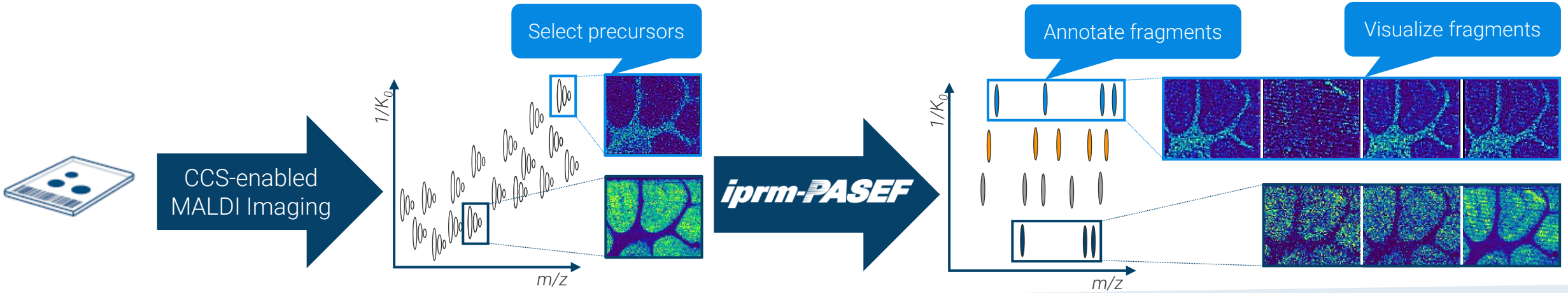
TC — prmPASEF acquisition

This Feature requires SCiLS Lab 2025a.

iprm-PASEF – identify your images with confidence!

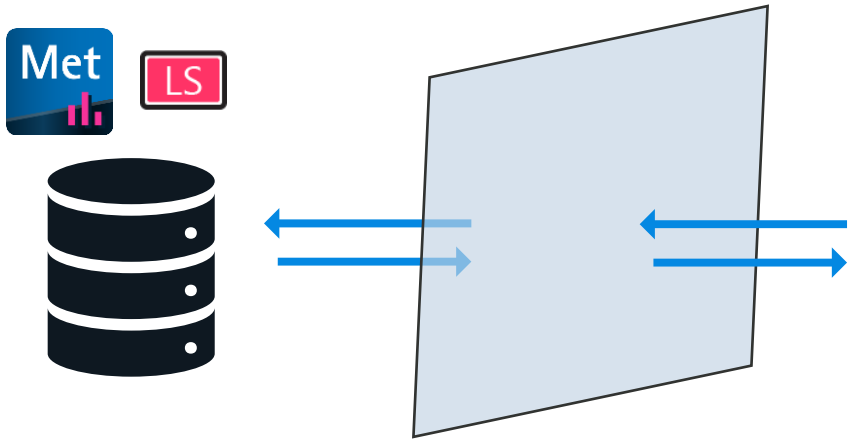
iprm-PASEF – identify your images with confidence

- Accurate MS/MS-based molecular identification
- 25 precursors in a single iprm-PASEF acquisition
- Integrated workflow: Acquire, Analyze & Annotate
  powered by timsTOF fleX, timsControl, SCiLS Lab & MetaboScape



REST API
Annotate your Features with Rule-Based Lipid Annotation

MetaboScape server



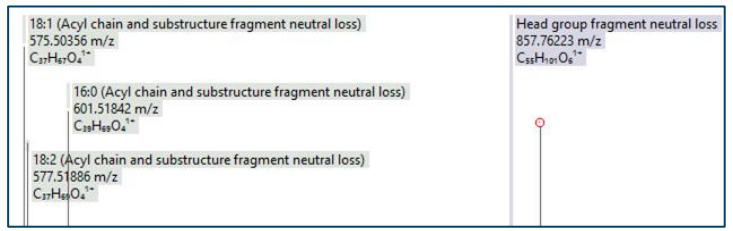
REST interface

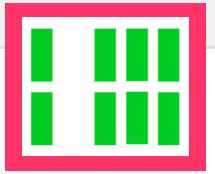
Your code:

Features

```
annotations = metaboscape_api.create_lipid_annotations_with_method
```

Scored annotations including fragment explanations

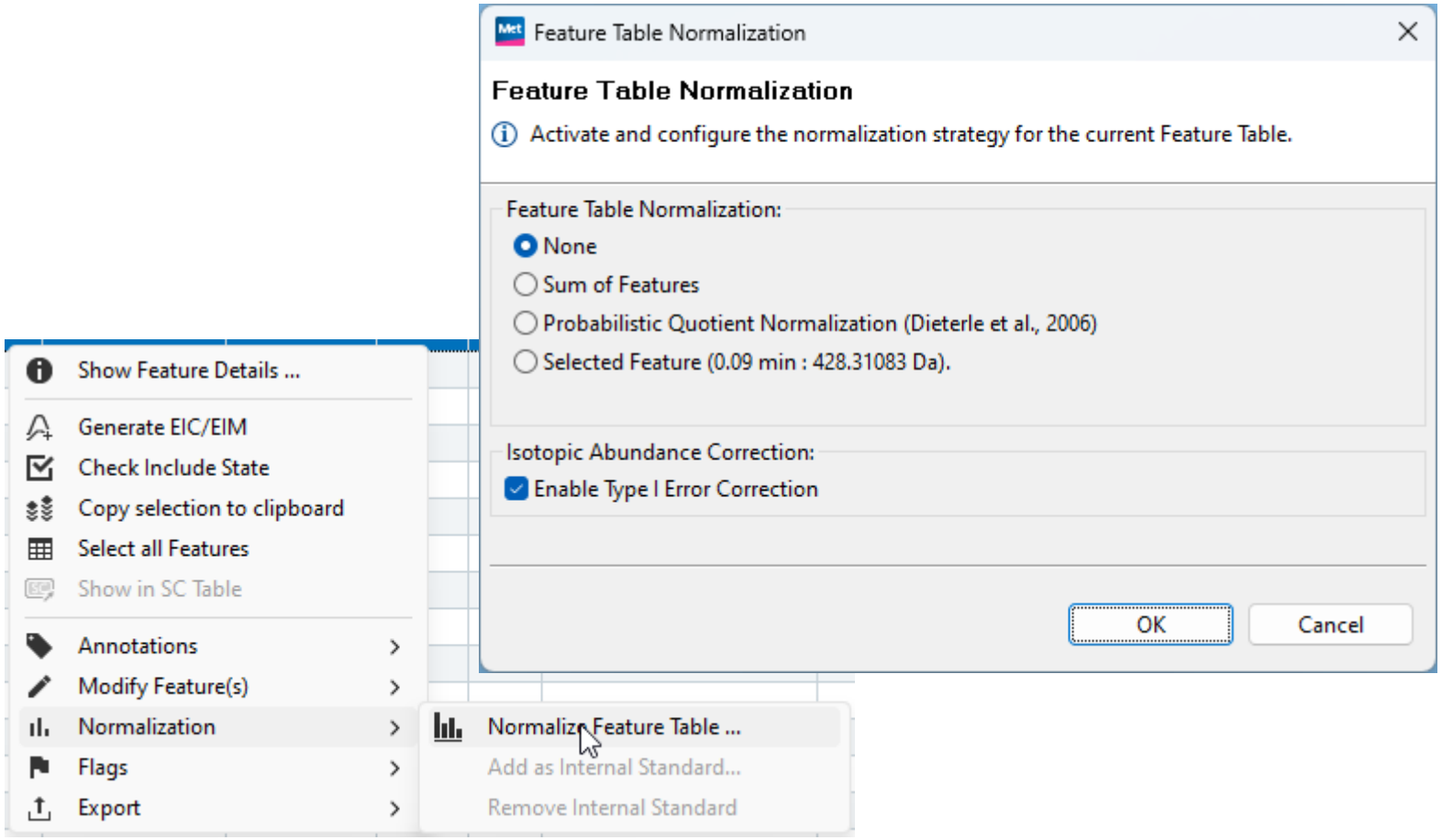


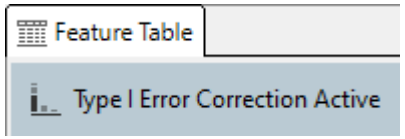


m/z value fit
Retention time fit
Isotopic pattern fit
MS/MS fit
CCS value fit

Use the full potential of the rule-based Lipid Species annotation algorithm including Annotation Quality scoring of up to four qualifiers (m/z, isotope patterns, MS/MS spectra, CCS values) to annotate lipid features in your own code.

Type-1 abundance error correction





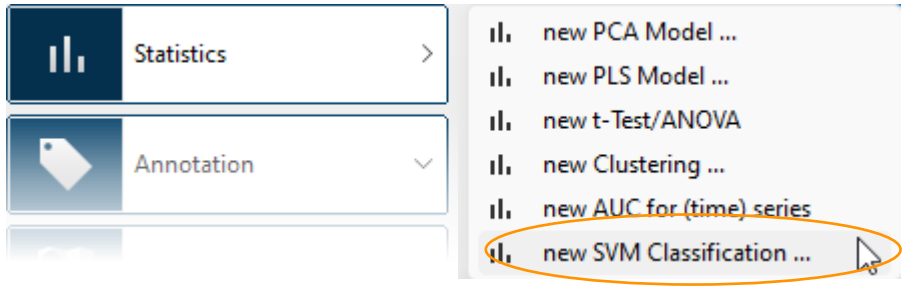
The relative amount of the total intensity of an ion, that is distributed across its naturally occuring isotopolgues, depends on its elemental composition. For instance, with each additional carbon atom in a molecule, due to naturally occurring ^{13}C atoms, the relative abundance of isotopologues increases while the relative abundance of the monoisotope decreases.

Especially in Lipidomics this „type 1 abdundance error" hampers internal standard normalization, as lipid class specific standards have to cover a range of different side chain lengths and thus different type 1 abundance errors.

The Lipidomics Standards Initiative (LSI) recommends correcting for type 1 abundance errors to ensure accurate quantitation.

➡ https://lipidomicstandards.org/lipid-species-quantification/ [23.07.2024]

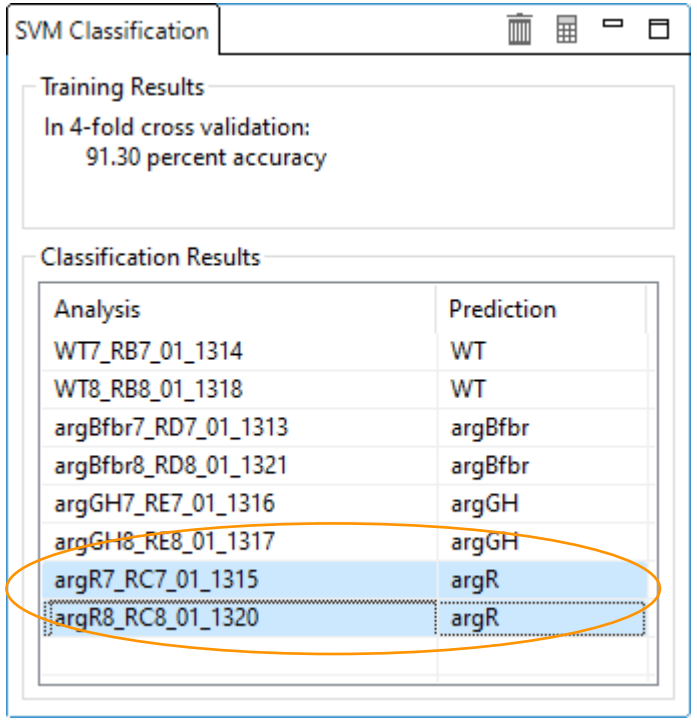
Support Vector Machine (SVM) Classification as Statistical View

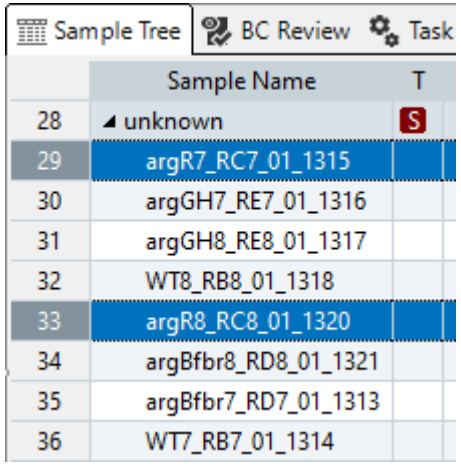


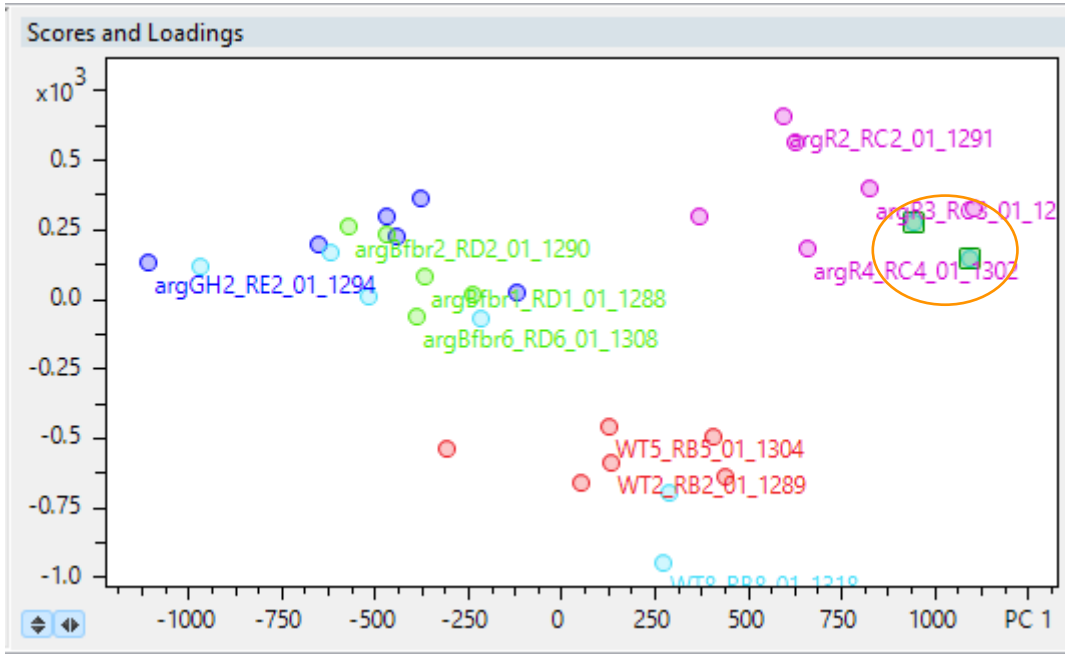
SVM Classification now is accessible through the Statistics menu and adds a new view to the bottom of the Overview perspective.

The classification will react to changes in the Include States of Analyses and Features.

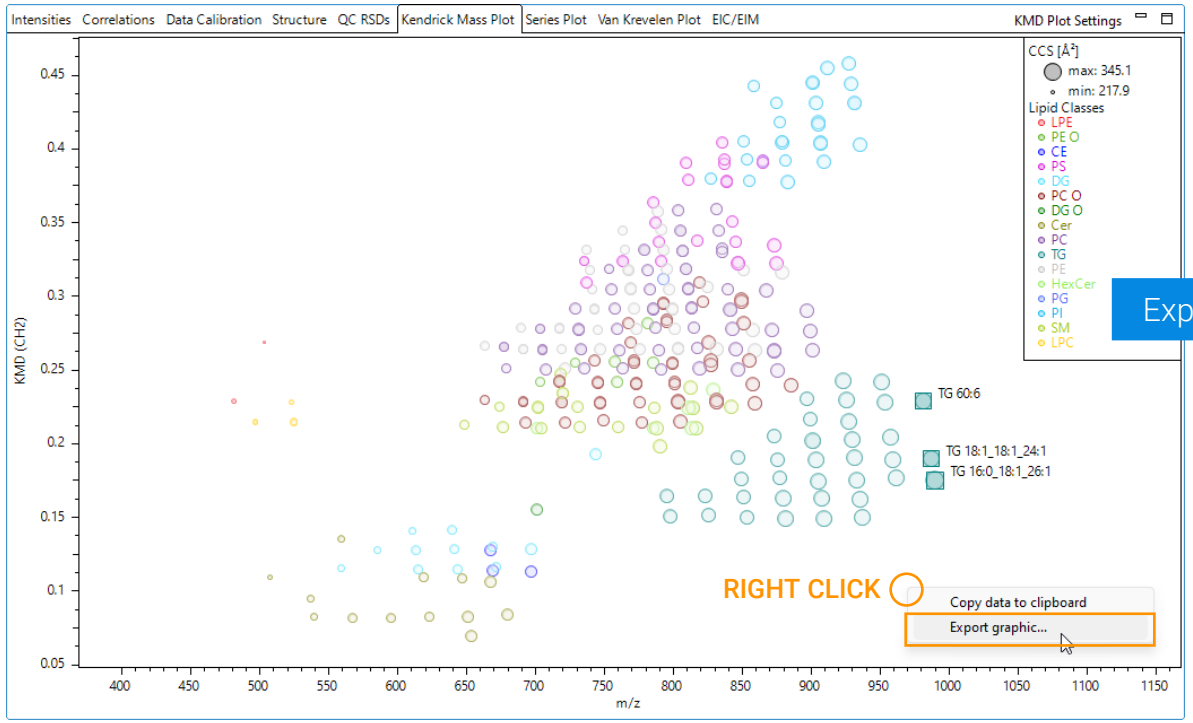
Selecting analyses from the Classification Results, will select them throughout the User Interface – for example in the Sample Tree and in other statistical views.





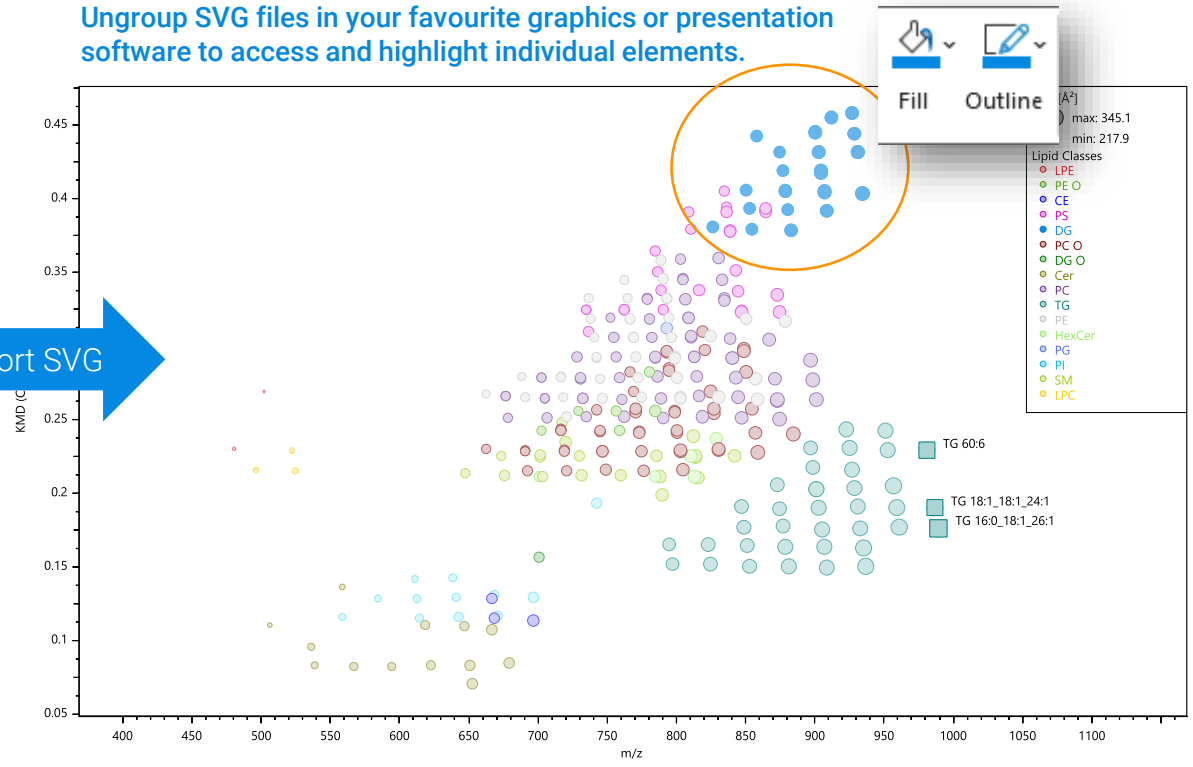


Export Kendrick Mass (Survey) plot into high quality graphics formats



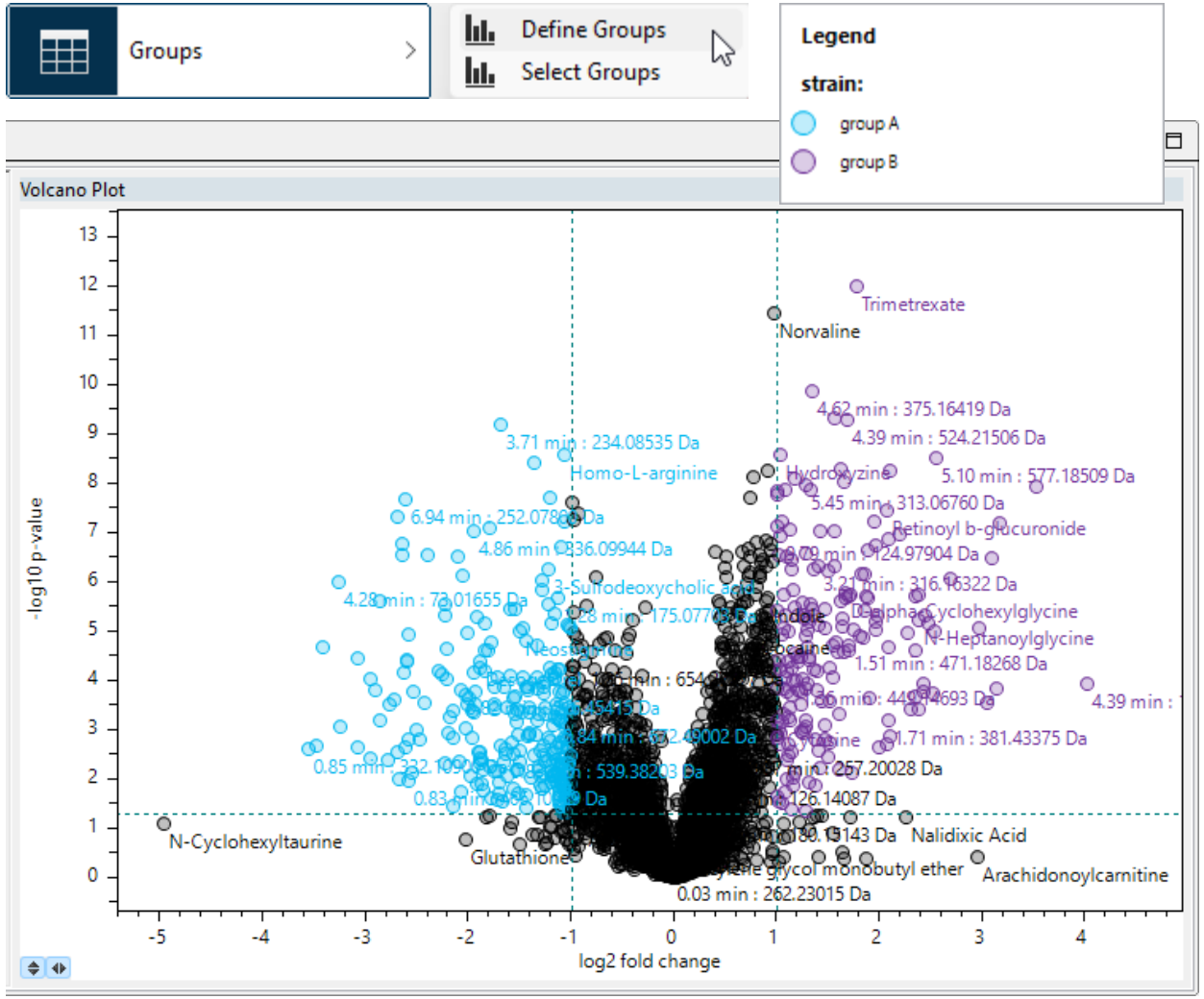
Export SVG

Ungroup SVG files in your favourite graphics or presentation software to access and highlight individual elements.



Export your Kendrick Mass (Survey) plot as you see it. The file formats SVG, PNG, EMF and GIF are available.
Especially SVG files are highly accessible in many graphics and presentation softwares and provide high quality for use in presentations and publications.

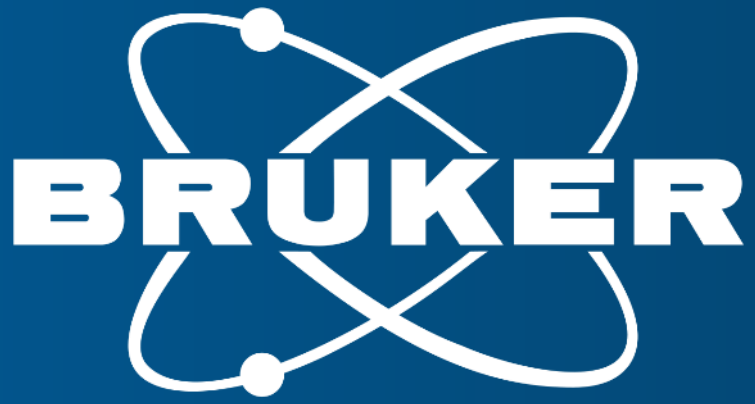
Volcano plot compound coloring according to statistical groups



The visualization of volcano plots now considers the colors assigned to the respective statistical groups.

In this example, the light blue compounds are more abundant in group A, while the purple compounds are more abundant in group B.

The volcano plot visualization can also be exported as SVG, PNG, EMF or GIF files.



Innovation with Integrity