What‘s new in MetaboScape 2023

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

Outline

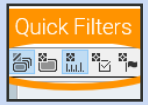
T-ReX 4D for timsTOF data: speed and peak picking improved

T-ReX² and T-ReX³ for imaging data use existing calibrations

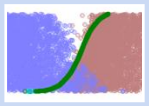
Processing and Annotation of Feature Tables in one go

Automatic CCS prediction for Spectral Libraries

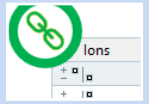
Outline



Feature Table quick filters



New means for data quality assessment



Smart-merge for positive and negative mode data

Improved response time for REST API

Miscellaneous

T-ReX 4D for timsTOF data: speed and peak picking improved

T-ReX 4D and T-ReX 3D

- Processing speed now about twice as fast when recursive extraction is active

T-ReX 4D

- Algorithmic improvement for rejection of false positive features
- Better computation of feature m/z values
- Improved computation of feature intensities
- Improved allocation of isotope patterns

T-ReX² and T-ReX³ for imaging data use existing calibrations

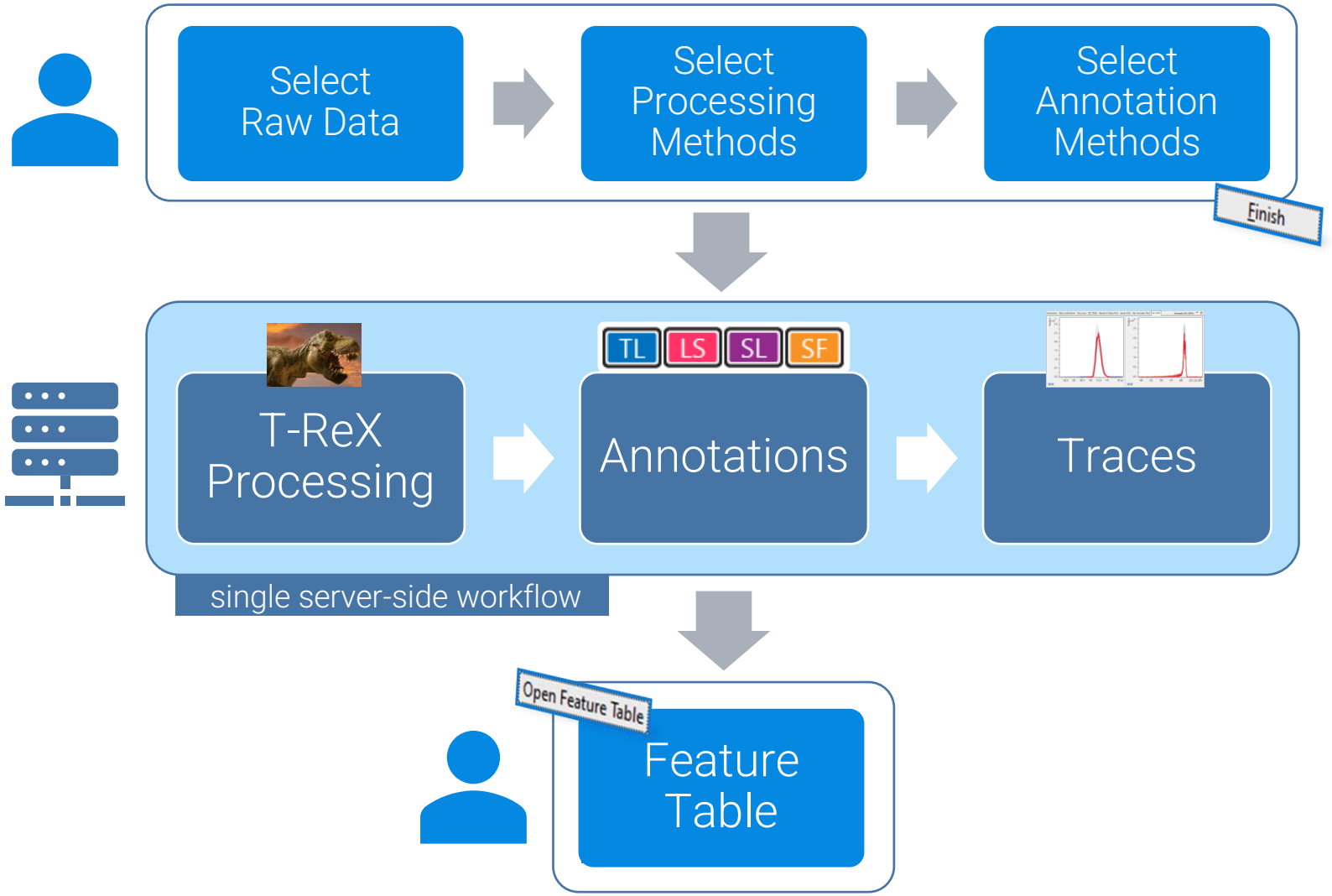
T-ReX² and T-ReX³ for imaging data now per default use the latest existing calibration available for the raw data.

This allows to use for example DataAnalysis to calibrate the data and the subsequent processing in MetaboScape will make use of it.

The same is true for the Bruker SCiLS Lab software, so that both use the same underlying calibration.

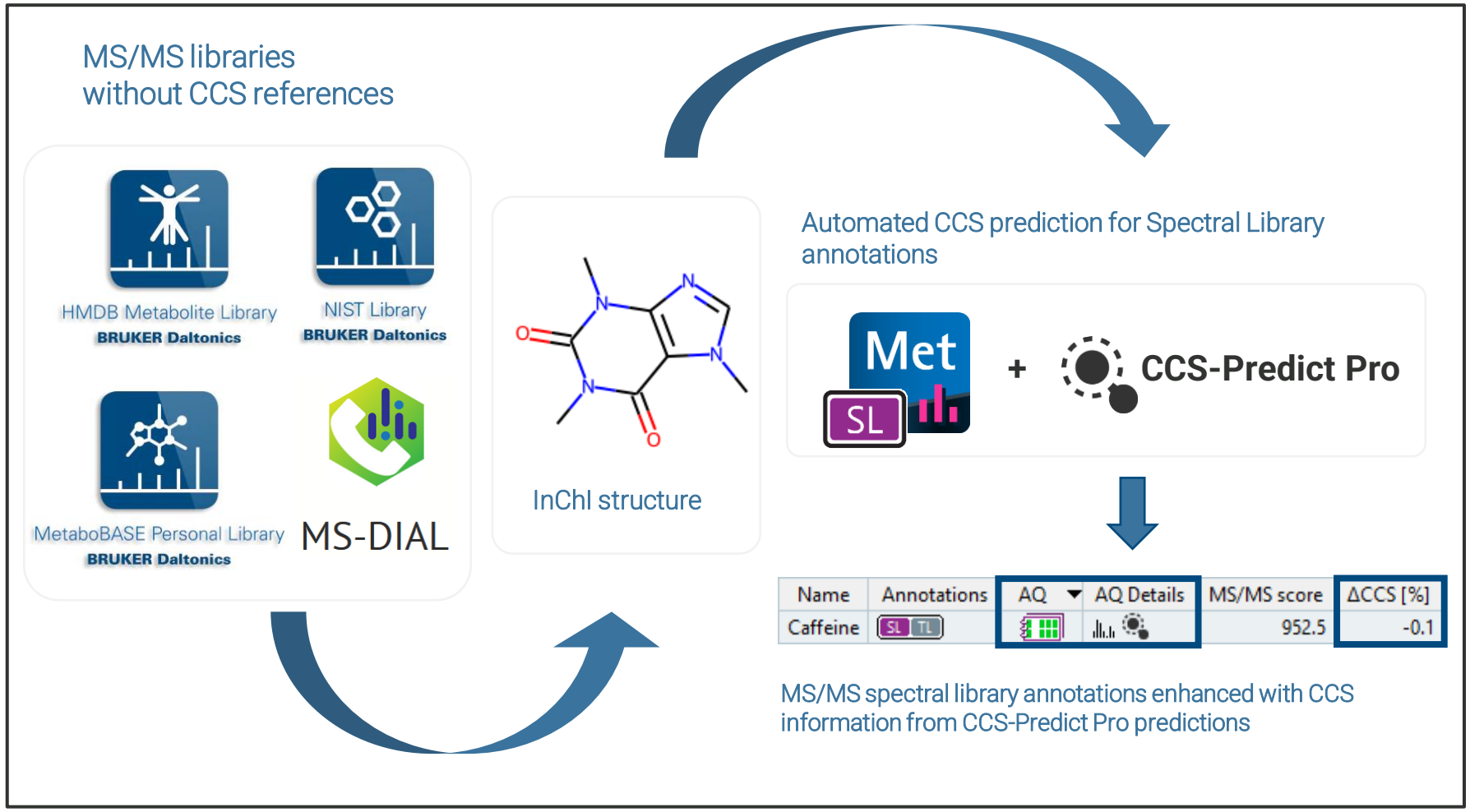
Processing and Annotation of Feature Tables in one go

Set up your Feature Table including data selection, processing methods and annotation methods **in one step**. The result will be a **fully processed and annotated Feature Table**. Additionally, for suitable data types EICs and EIMs will automatically be generated for all features annotated by Target List, Lipid Species, or Spectral Library.



Automatic CCS prediction for Spectral Libraries

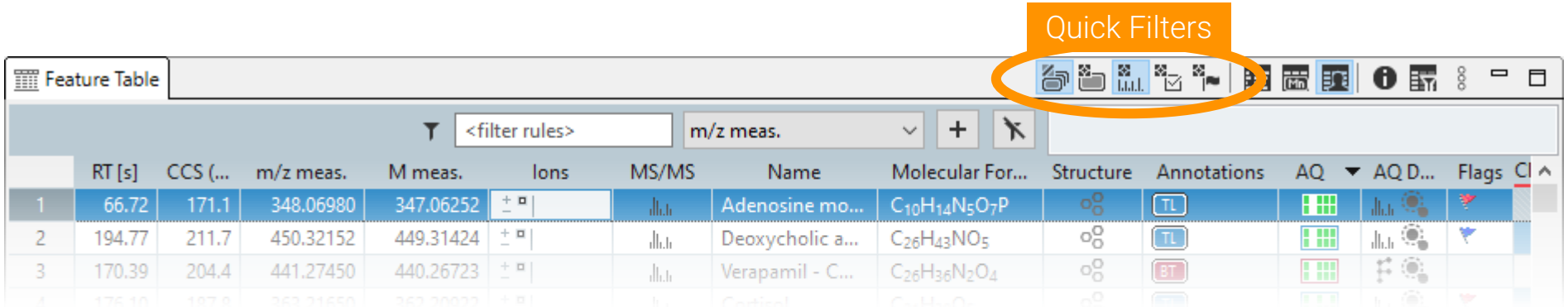
The novel CCS-Predict workflow in MetaboScape turns any MS/MS spectral library with structure information into a CCS-enabled library. It automatically calculates CCS-based annotation quality scores and labels predicted values in the Annotation Quality (AQ) Details column.



Feature Table Quick Filters

The new Quick Filters allow to narrow down the Feature Table with a single click.

Quick Filters can be freely combined with the other filter rules, allowing for easy configuration of complex filter settings.



Hide duplicate annotations
If multiple Features are annotated with the same name show only the most reliably found and matched one.

Show only annotated Features

Show only Features with attached MS/MS spectrum

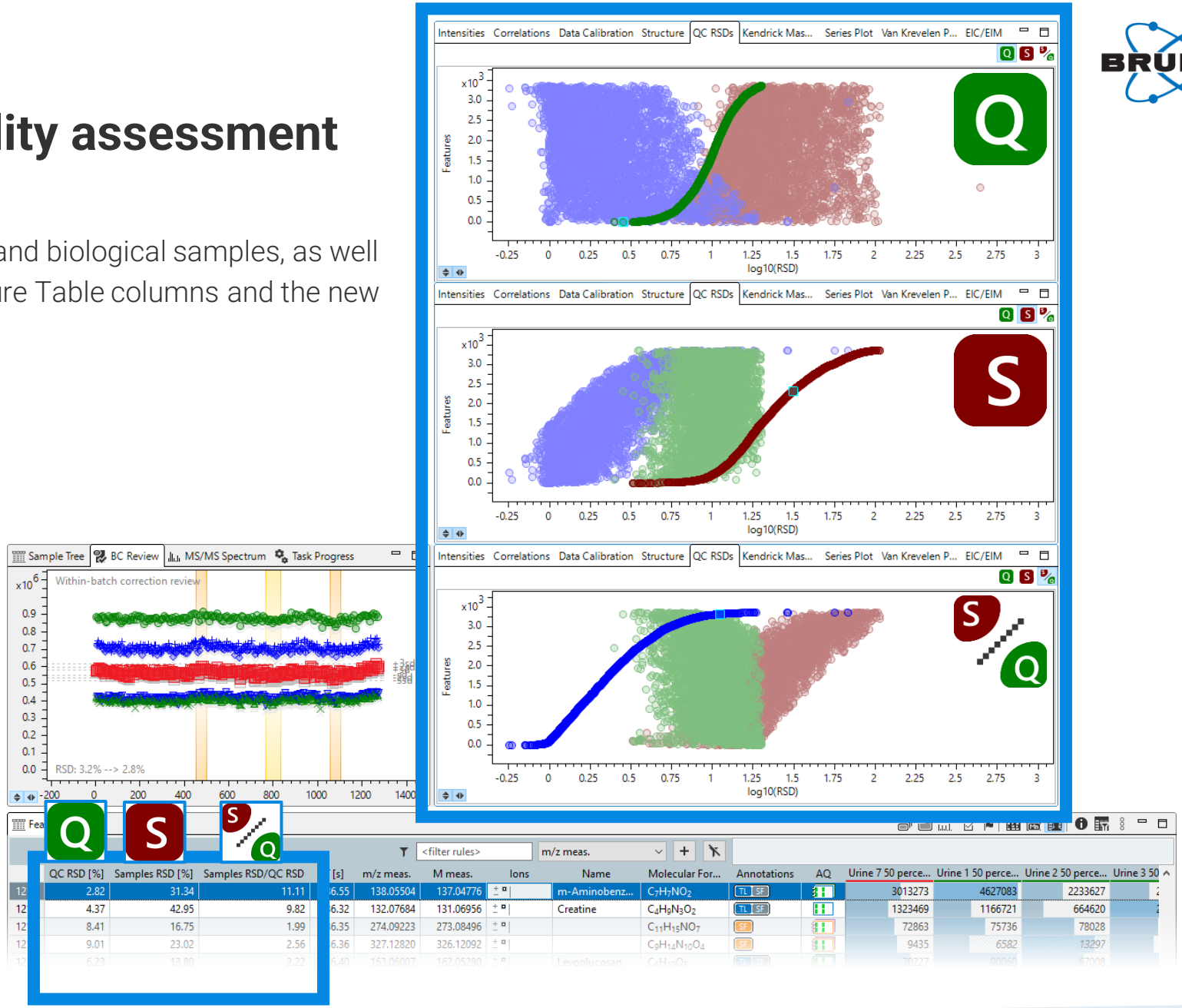
Show only Features that are included for statistics

Show only flagged Features

New means for data quality assessment

Assess relative standard deviations in QCs and biological samples, as well as the quotient of both, using the new Feature Table columns and the new QC RSDs plot.

- %RSD in quality control samples
- %RSD in biological samples
- The quotient of RSDs in biological samples and quality control samples



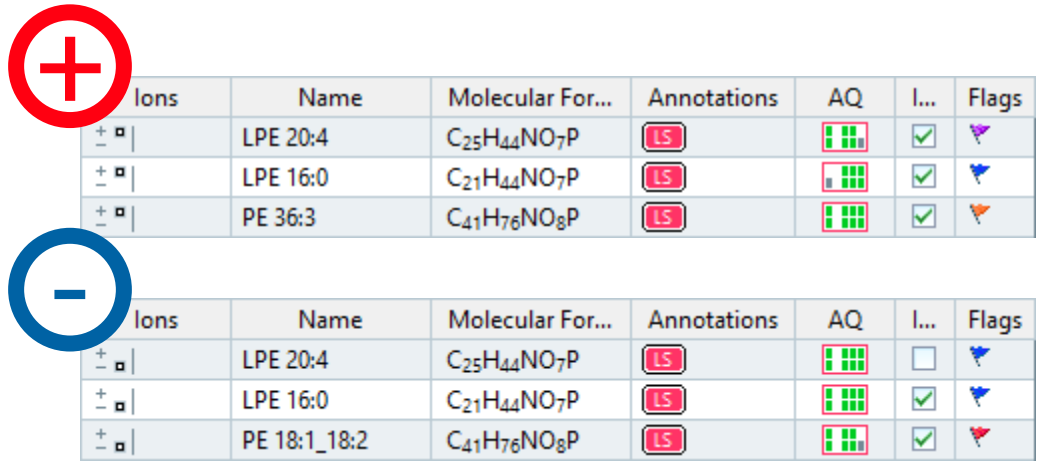
Lewis, Matthew R et al. "Development and Application of Ultra-Performance Liquid Chromatography-TOF MS for Precision Large Scale Urinary Metabolic Phenotyping." *Analytical chemistry* vol. 88,18 (2016): 9004-13. doi:10.1021/acs.analchem.6b01481

Smart merging for positive and negative mode data

Merging of positive- and negative-mode Feature Tables now follows new rules to preserve the best possible annotations of the two modes. The new rule set to determine the new primary ion of the merged Feature is listed to the right.

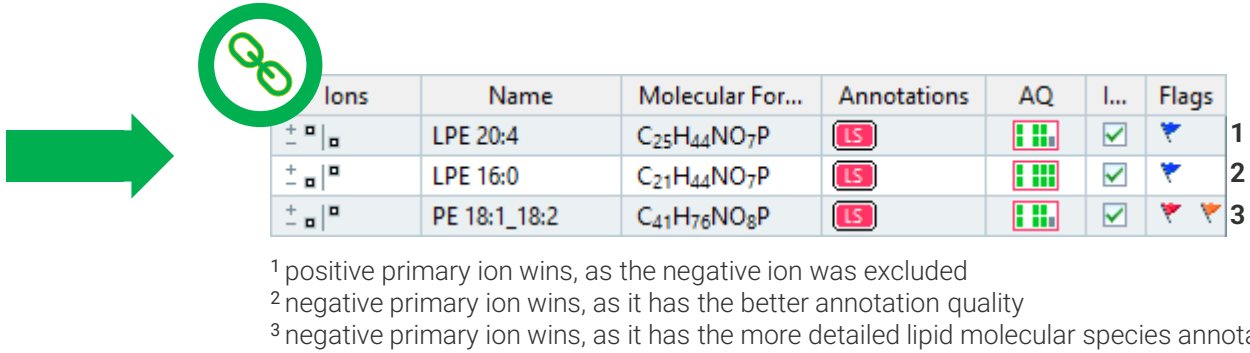
Additionally, the Include state for statistics (the checkbox) as well as Flags are now transferred into the merged Feature Table.

The below example shows how Lipid (Molecular) Species Level and AQ decide over the primary ion of the merged feature table. It is also visible, how the Include state is considered and how Flags are combined from both polarities.



Ions	Name	Molecular For...	Annotations	AQ	I...	Flags
[M+H]+	LPE 20:4	$C_{25}H_{44}NO_7P$	LS		☑	
[M+H]+	LPE 16:0	$C_{21}H_{44}NO_7P$	LS		☑	
[M+H]+	PE 36:3	$C_{41}H_{76}NO_8P$	LS		☑	

Ions	Name	Molecular For...	Annotations	AQ	I...	Flags
[M-H]-	LPE 20:4	$C_{25}H_{44}NO_7P$	LS		☐	
[M-H]-	LPE 16:0	$C_{21}H_{44}NO_7P$	LS		☑	
[M-H]-	PE 18:1_18:2	$C_{41}H_{76}NO_8P$	LS		☑	



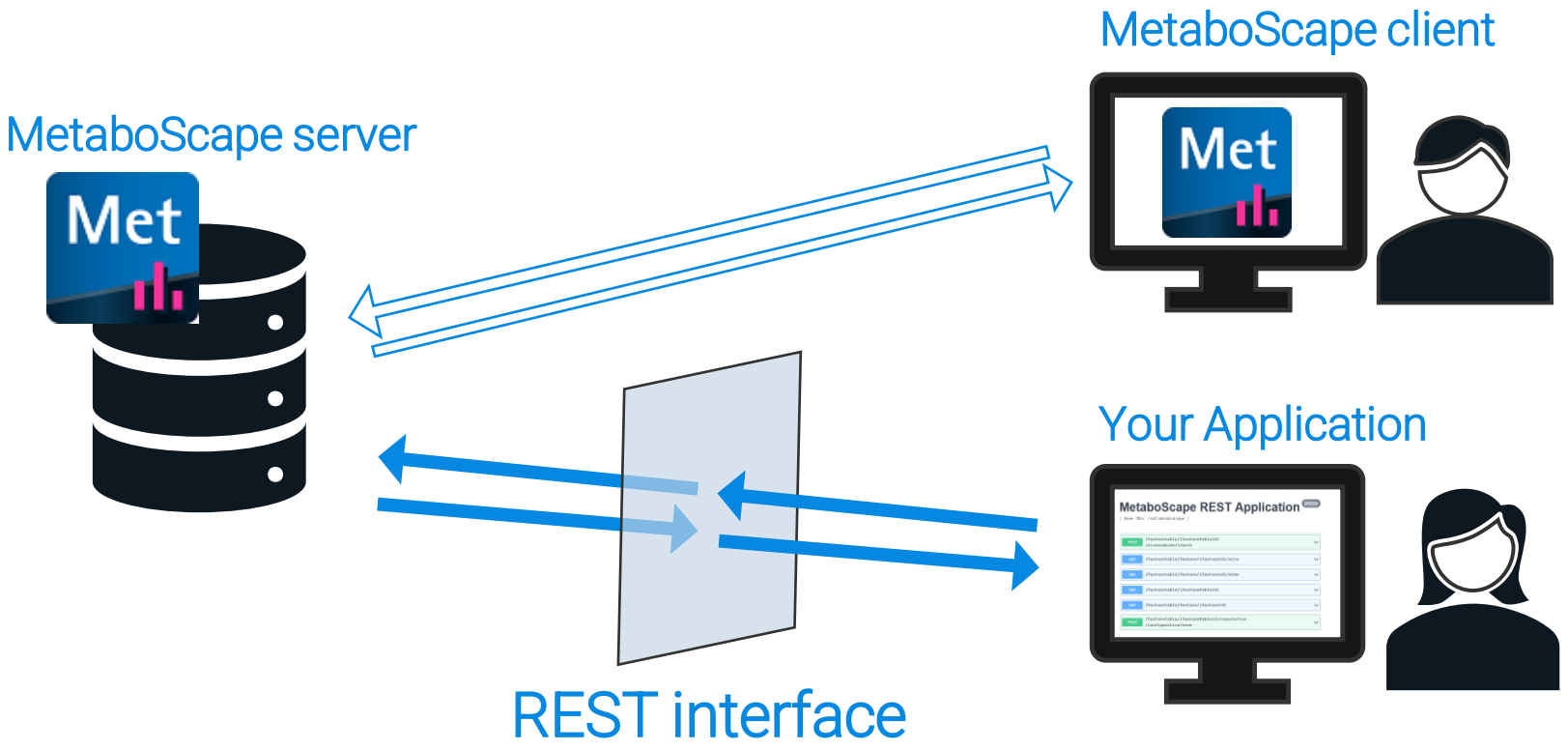
Ions	Name	Molecular For...	Annotations	AQ	I...	Flags	
[M+H]+	LPE 20:4	$C_{25}H_{44}NO_7P$	LS		☑		1
[M-H]-	LPE 16:0	$C_{21}H_{44}NO_7P$	LS		☑		2
[M-H]-	PE 18:1_18:2	$C_{41}H_{76}NO_8P$	LS		☑		3

[1] positive primary ion wins, as the negative ion was excluded
[2] negative primary ion wins, as it has the better annotation quality
[3] negative primary ion wins, as it has the more detailed lipid molecular species annotation

New Merging Rule Set

1. Included over Excluded
2. Annotated over not-annotated
3. Higher annotation tool over lower
4. For Lipid Species annotations: Molecular Species level over Species level
5. AQ Symbol
6. AQ Raw scores
7. Intensity

Improved response time for REST API



Each REST call now will be processed faster by the MetaboScape server, so that especially scripts which send multiple subsequent requests to the REST API will run significantly faster.

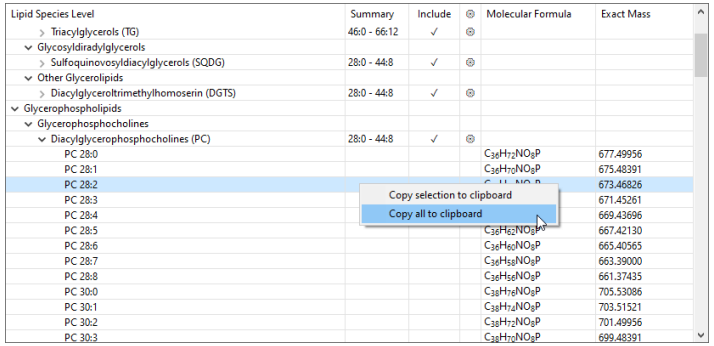
Miscellaneous

Version Update Notifications

When there is a new version of MetaboScape, the software will let you know once you log in. The pop up notification will come with a link to our download website.

Copy Lipid Species Tree from Annotation Method

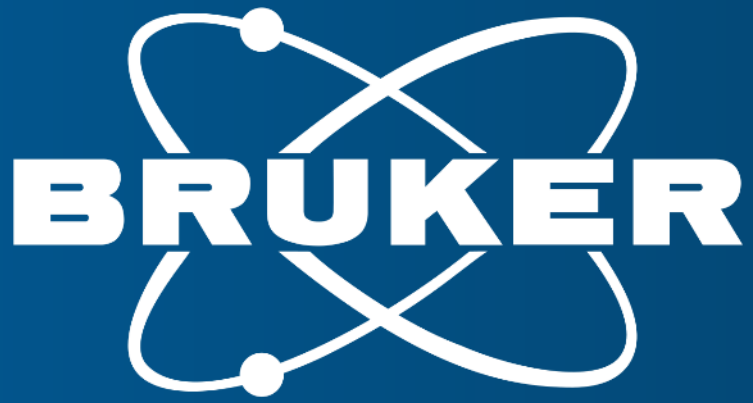
A new context menu in the Lipid Species annotation method allows you to copy the tree of lipid species you have configured. From your clipboard you can then paste it into a spreadsheet, for example.



Mobility calibration summary in Sample Tree

Find the standard deviation of mobility calibration residuals ($1/K_0$ x 1000) in the Sample Tree for a quick quality check.

Mass Calib...	Chrom. Align. ...	Mob. calibr.
0.140	0.15288	6.349
0.063	0.49605	5.962
0.105	0.07093	6.390
0.182	0.11006	7.365
0.119	0.06402	6.473
0.174	0.09643	5.875



Innovation with Integrity