What’s new in MetaboScape® 2025b

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

Outline

01 Homologous Series Extension

02 dda-PASEF® to Fluxomics in TASQ®

03 dda-PASEF to prm-PASEF®
4D-Lipidomics; monitor isomeric species

04 Spectral Library: Tolerance-based Matching and improved import

05 Improved UI for *in-silico* derivatization methods

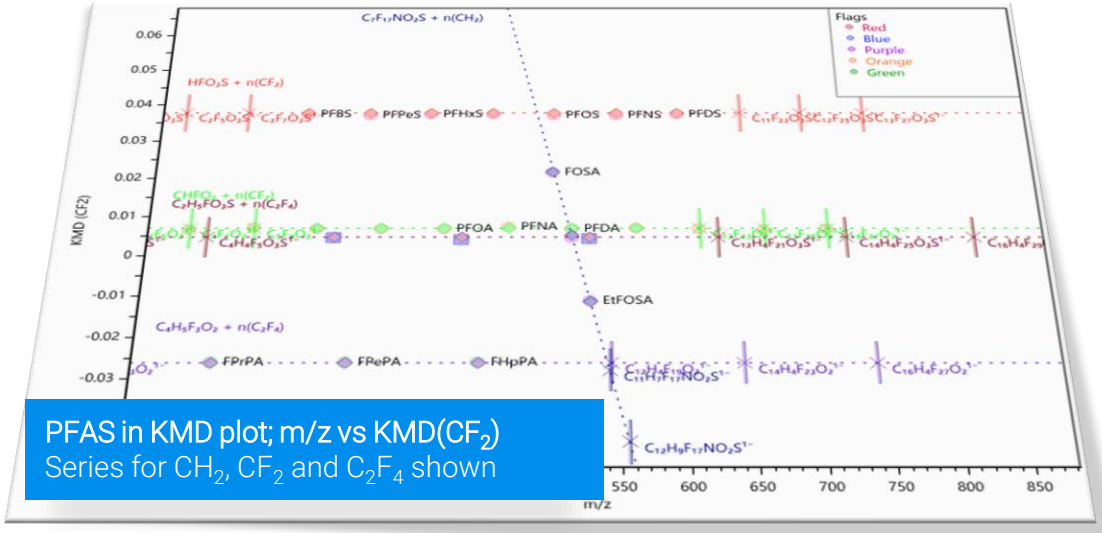
06 Streamlined use of Flags

07 New Survey Plot color modes

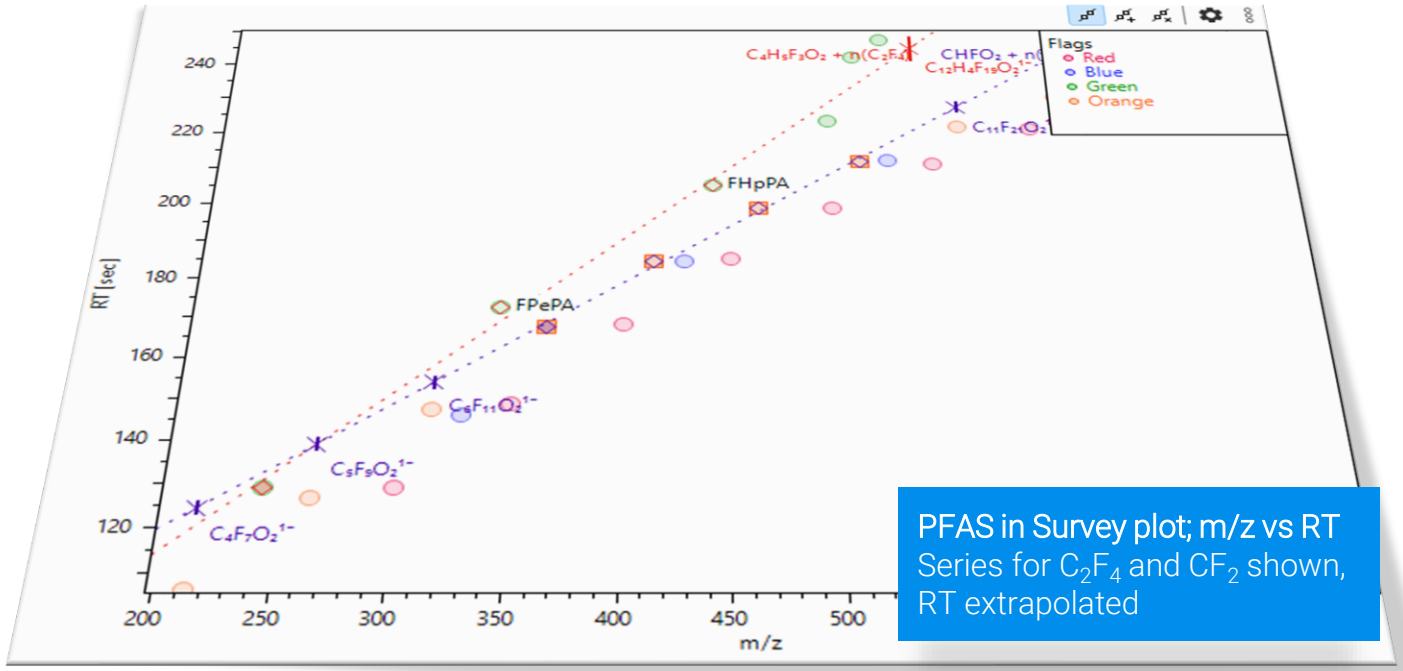
08 REST API: Annotate with SmartFormula

Homologous Series Extension

Select annotated features of a homologous series, to extrapolate the series and mark positions of potential further members of that series.



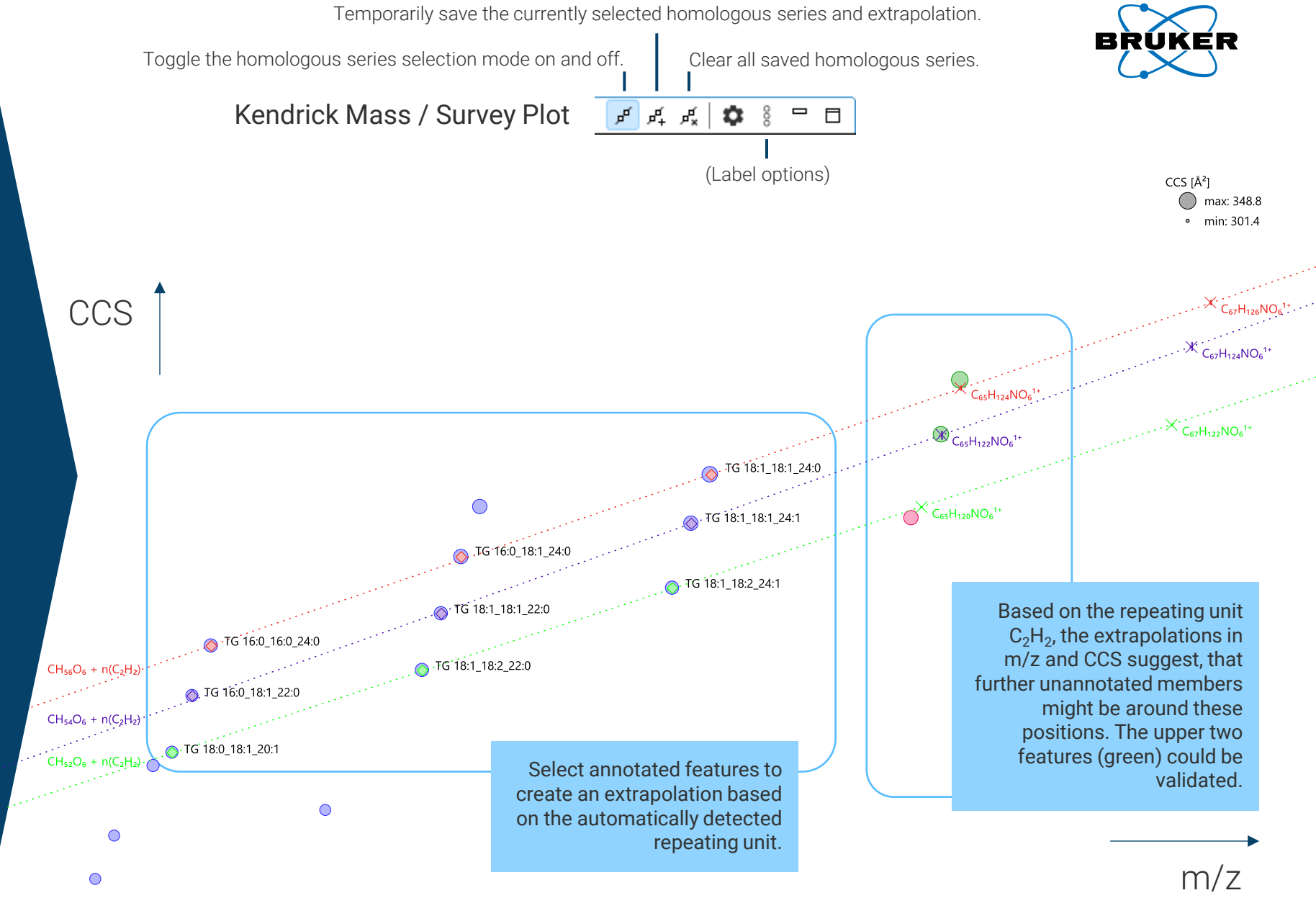
PFAS in KMD plot; m/z vs KMD(CF_2)
Series for CH_2, CF_2 and C_2F_4 shown



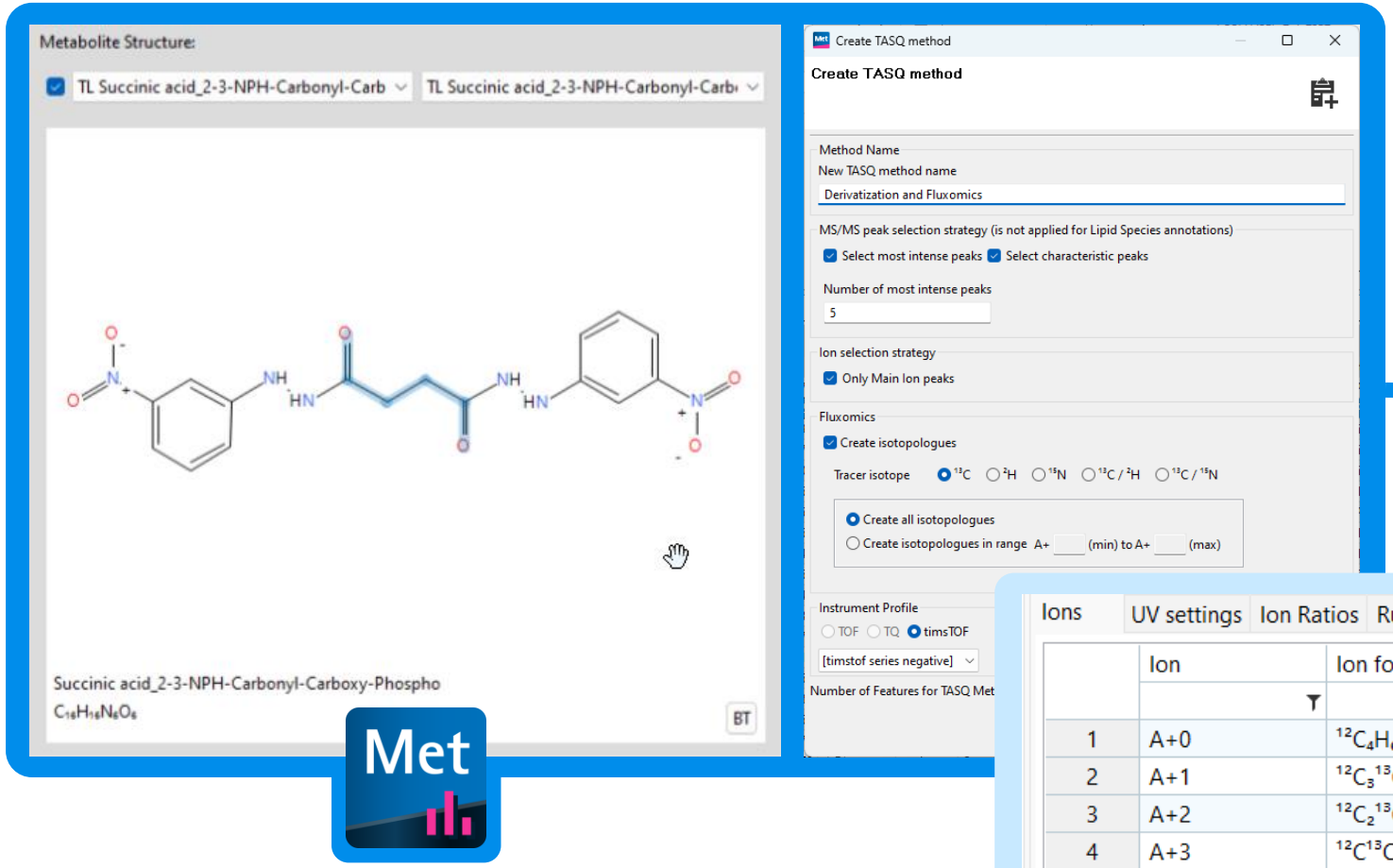
PFAS in Survey plot; m/z vs RT
Series for C_2F_4 and CF_2 shown, RT extrapolated

Homologous Series Extension

Select annotated features of a homologous series, to extrapolate the series and mark positions of potential further members of that series.



dda-PASEF to Fluxomics
From MetaboScape to TASQ



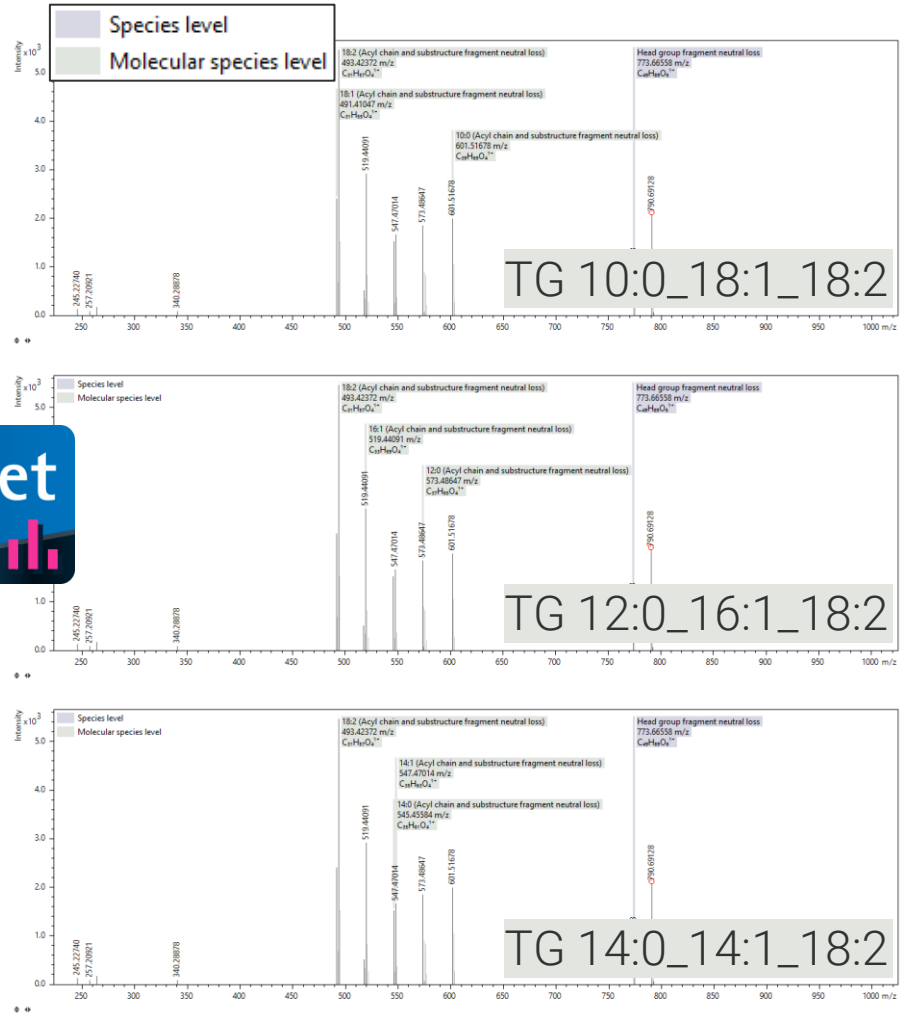
Create TASQ Fluxomics methods from within MetaboScape. Create ^{13}C or other isotopologues based on the respective ^{12}C species found in MetaboScape. For in-silico derivatization experiments, the isotopologue generation automatically focuses on the remainder of the original (underivatized) metabolites, and spares atoms that stem from the derivatization agent. Compare blue structure highlight in the structure view on the left to the list of generated isotopologues in the bottom. See TASQ for more information on the Fluxomics workflow.

ASQ

Ions | UV settings | Ion Ratios | Rules

	Ion	Ion formula	m/z	Spectrum type	Mandatory	Quant. ion
1	A+0	$^{12}C_4H_6ClO_4^{1-}$	152.9960	FullScan	☑	☑
2	A+1	$^{12}C_3{}^{13}CH_6ClO_4^{1-}$	153.9994	FullScan	☐	☐
3	A+2	$^{12}C_2{}^{13}C_2H_6ClO_4^{1-}$	155.0027	FullScan	☐	☐
4	A+3	$^{12}C^{13}C_3H_6ClO_4^{1-}$	156.0061	FullScan	☐	☐
5	A+4	$^{13}C_4H_6ClO_4^{1-}$	157.0094	FullScan	☐	☐

dda-PASEF to prm-PASEF
Monitoring transitions of multiple isomeric Lipid Species



Head group fragment neutral loss
773.66558 m/z
$C_{49}H_{89}O_6^{1+}$

10:0 (Acyl chain and substructure fragment neutral loss)
601.51678 m/z
$C_{39}H_{69}O_4^{1+}$

12:0 (Acyl chain and substructure fragment neutral loss)
573.48647 m/z
$C_{37}H_{65}O_4^{1+}$

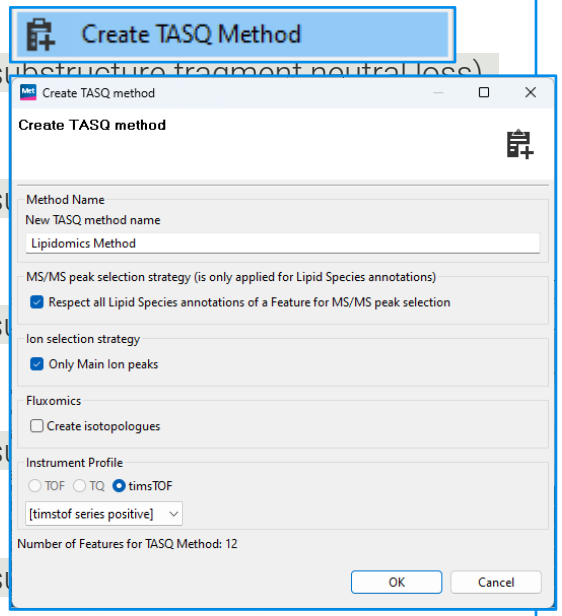
14:1 (Acyl chain and substructure fragment neutral loss)
547.47014 m/z
$C_{35}H_{63}O_4^{1+}$

14:0 (Acyl chain and substructure fragment neutral loss)
545.45584 m/z
$C_{35}H_{61}O_4^{1+}$

16:1 (Acyl chain and substructure fragment neutral loss)
519.44091 m/z
$C_{33}H_{59}O_4^{1+}$

18:2 (Acyl chain and substructure fragment neutral loss)
493.42372 m/z
$C_{31}H_{57}O_4^{1+}$

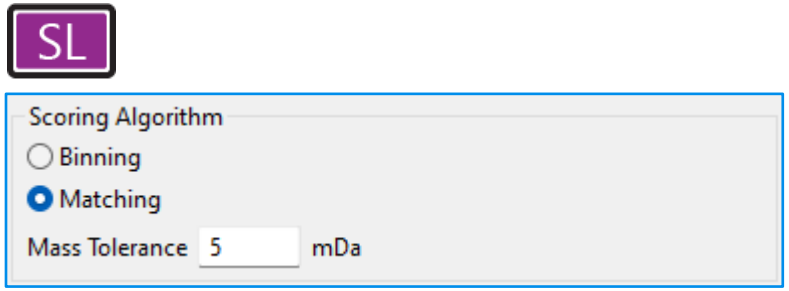
18:1 (Acyl chain and substructure fragment neutral loss)
491.41047 m/z
$C_{31}H_{55}O_4^{1+}$



From within MetaboScape, create TASQ methods to inform prm-PASEF. Set up parallel reaction monitoring for characteristic side chain fragments of coeluting isomeric lipid species.

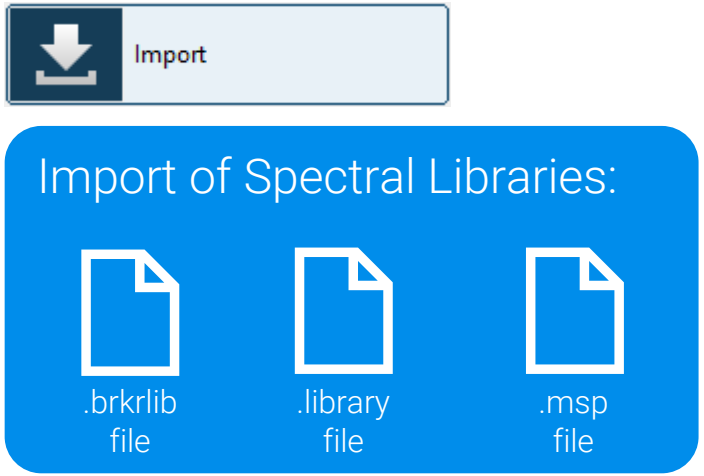
Spectral Library Improvements: Matching Algorithm and Import Performance

New Matching Algorithm replaces Binning



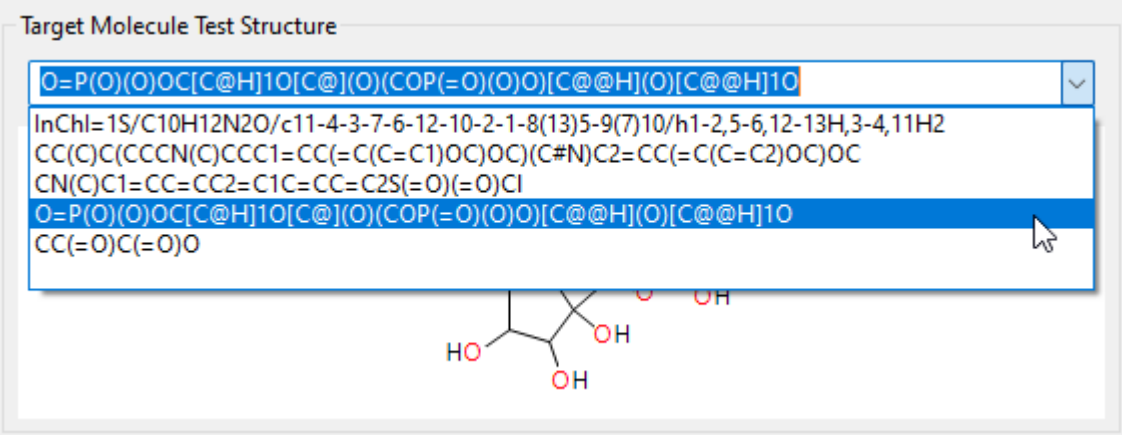
The Spectral Library annotation tool uses cosine scores to assess matches between measured and reference spectra. Now a mass tolerance-based matching algorithm is used to associate the respective signals from both spectra and replaces the former binning algorithm. This change results in a more reliable and intuitive association of mass signals, leading to more representative scoring.

Faster, non-UI-blocking Library Import

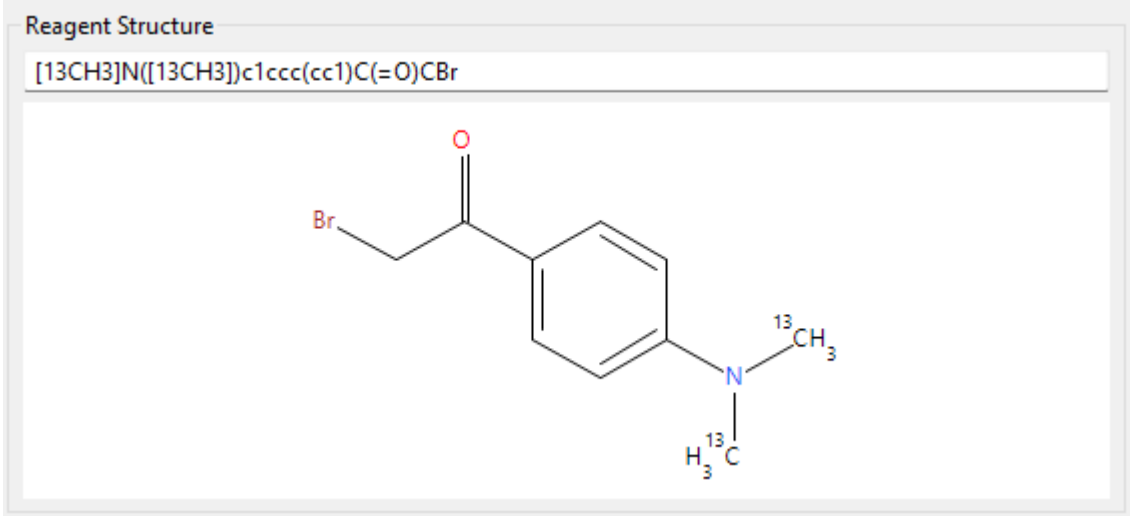


The import of the Spectral Library has been enhanced to run as a server task. This improvement not only boosts performance but, more importantly, ensures that the client user interface remains unblocked during the import.

Improved UI for *in-silico* derivatization methods



Efficiently switch between your favourite test structures for you in-silico derivatization methods: Your last used structures are remembered, so that you can easily switch between structures to test your method for different functional groups.

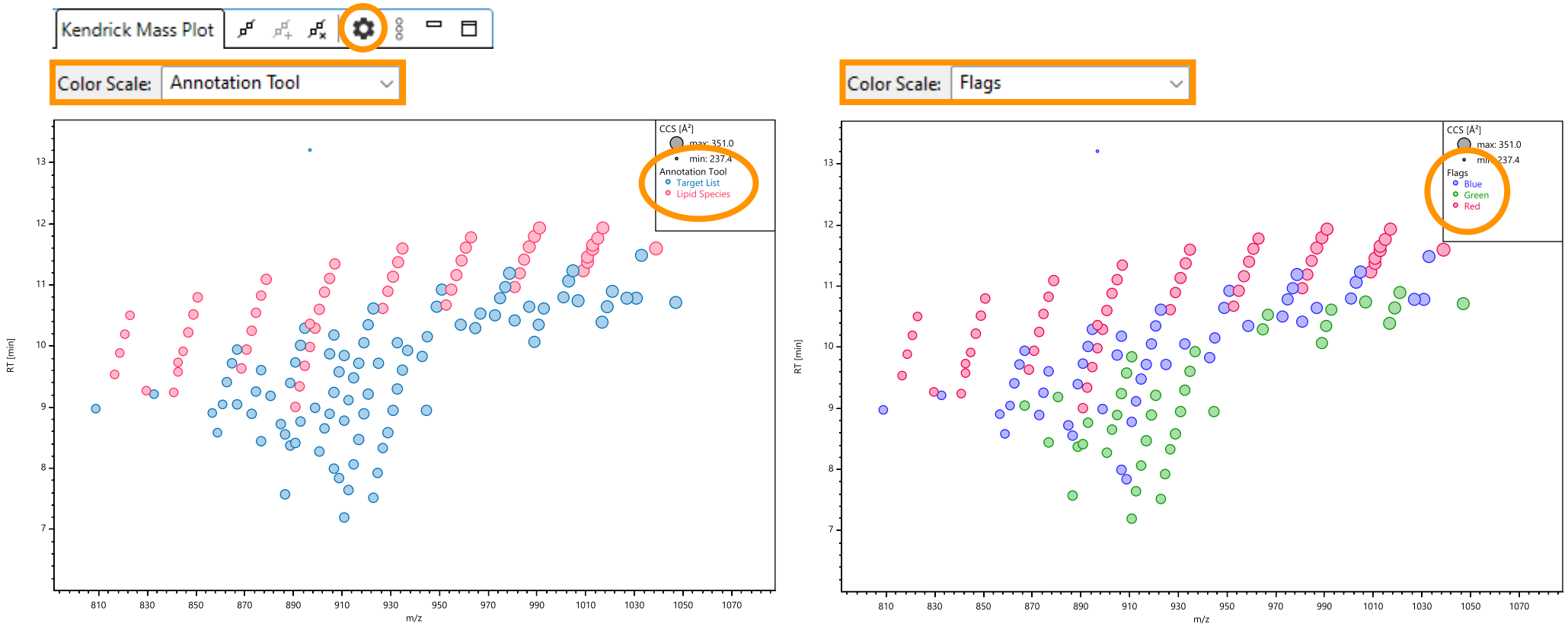


The in-silico derivatization user interface now also allows to validate methods designed for use with isotopically labelled derivatization reagents. Here, DmpA with two ^{13}C atoms is used. In MetaboScape 2025b, isotopically labelled compounds require to turn off MetFrag *in-silico* fragmentation.

This Feature requires a dedicated software license.

Please refer to the "What's New in MetaboScape 2025" document for further information *on in-silico* derivatization and how to unlock the Feature in MetaboScape 2025 or later.

New Color Modes for the KMD / Survey Plot: Annotation Tool and Flags

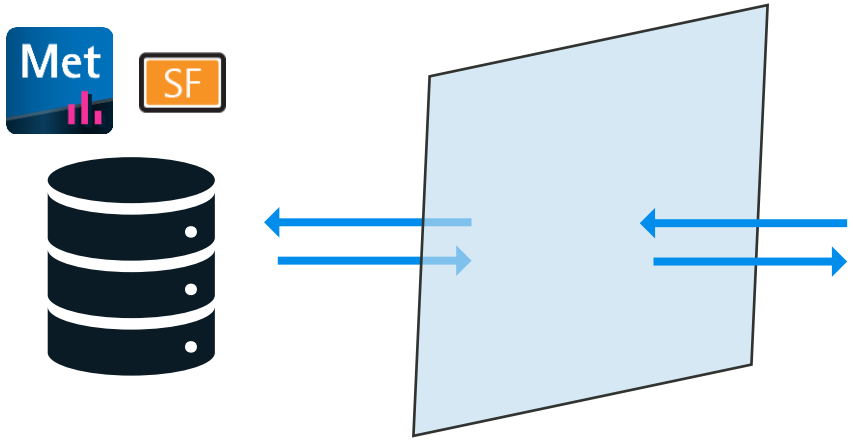


The new Color Scale options in the Kendrick Mass Plot / Survey View enable users to highlight features based on the annotation tools used or their first flag color. In the examples above, the left image shows TG lipids annotated with the Lipid Species tool, while further oxidized TGs were identified using a dedicated Target List. In the right image, red, blue, and green flags indicate TGs that are unoxidized, oxidized once, and oxidized twice, respectively.

REST API
Annotate your Features with SmartFormula

Apply MetaboScape's SmartFormula, including it's metabolomics-tailored rule sets, within your own bioinformatics pipelines.

MetaboScape server



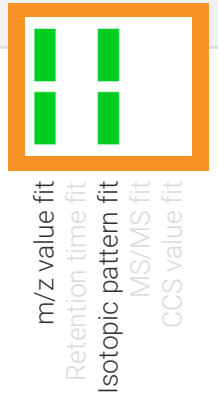
REST interface

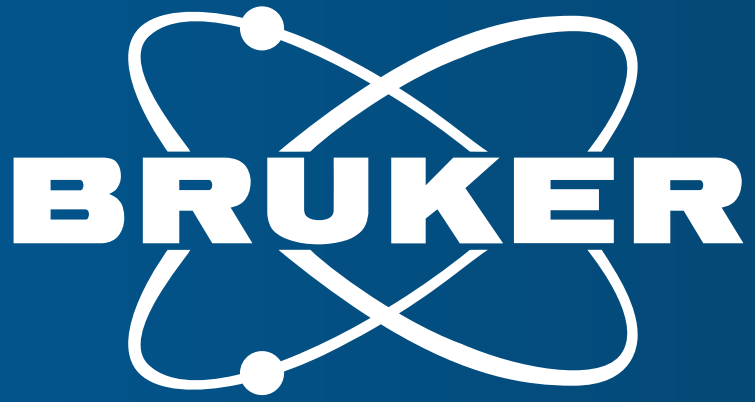
Your code:

Features

```
annotations = metaboscape_api.create_smartformula_annotations_with_method
```

Scored annotations based on m/z and isotope pattern fit.





Innovation with Integrity