

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

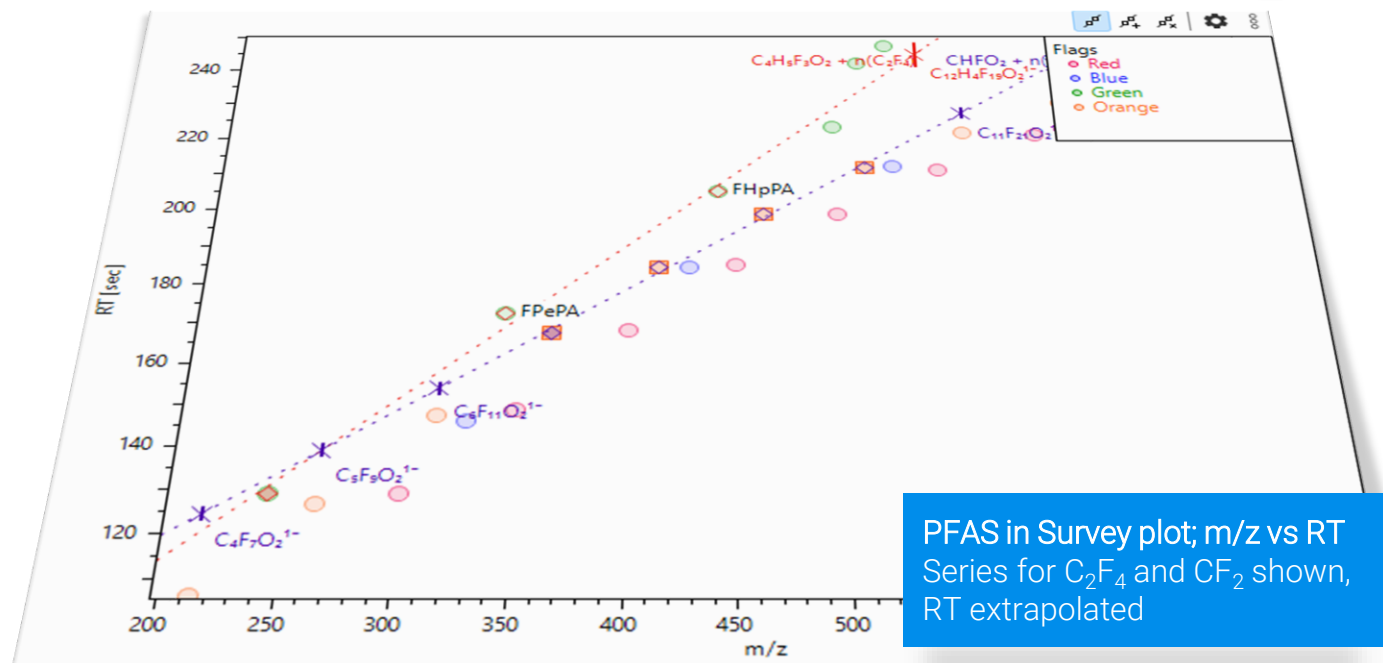
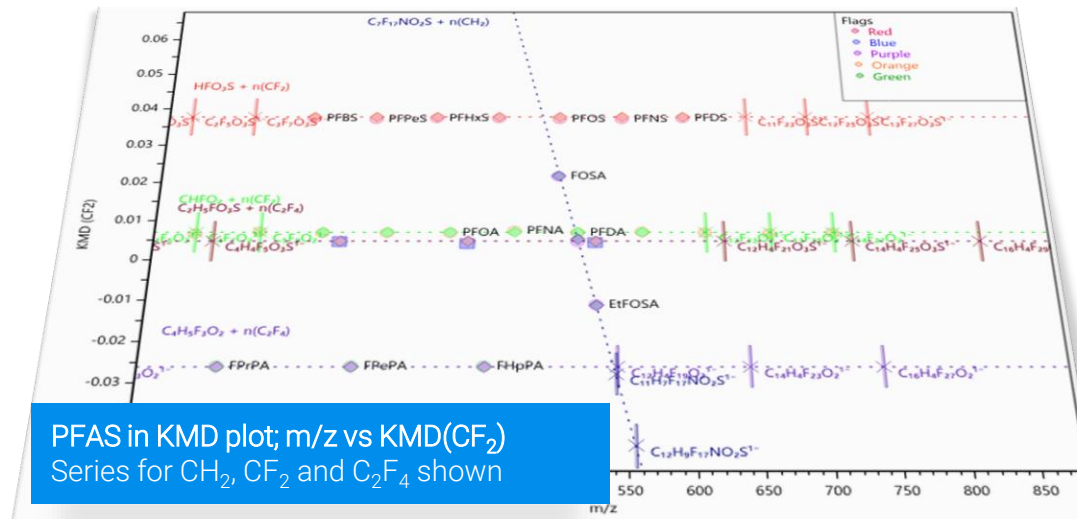


Outline

- 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.



Temporarily save the currently selected homologous series and extrapolation.



Toggle the homologous series selection mode on and off.

Clear all saved homologous series.

Kendrick Mass / Survey Plot

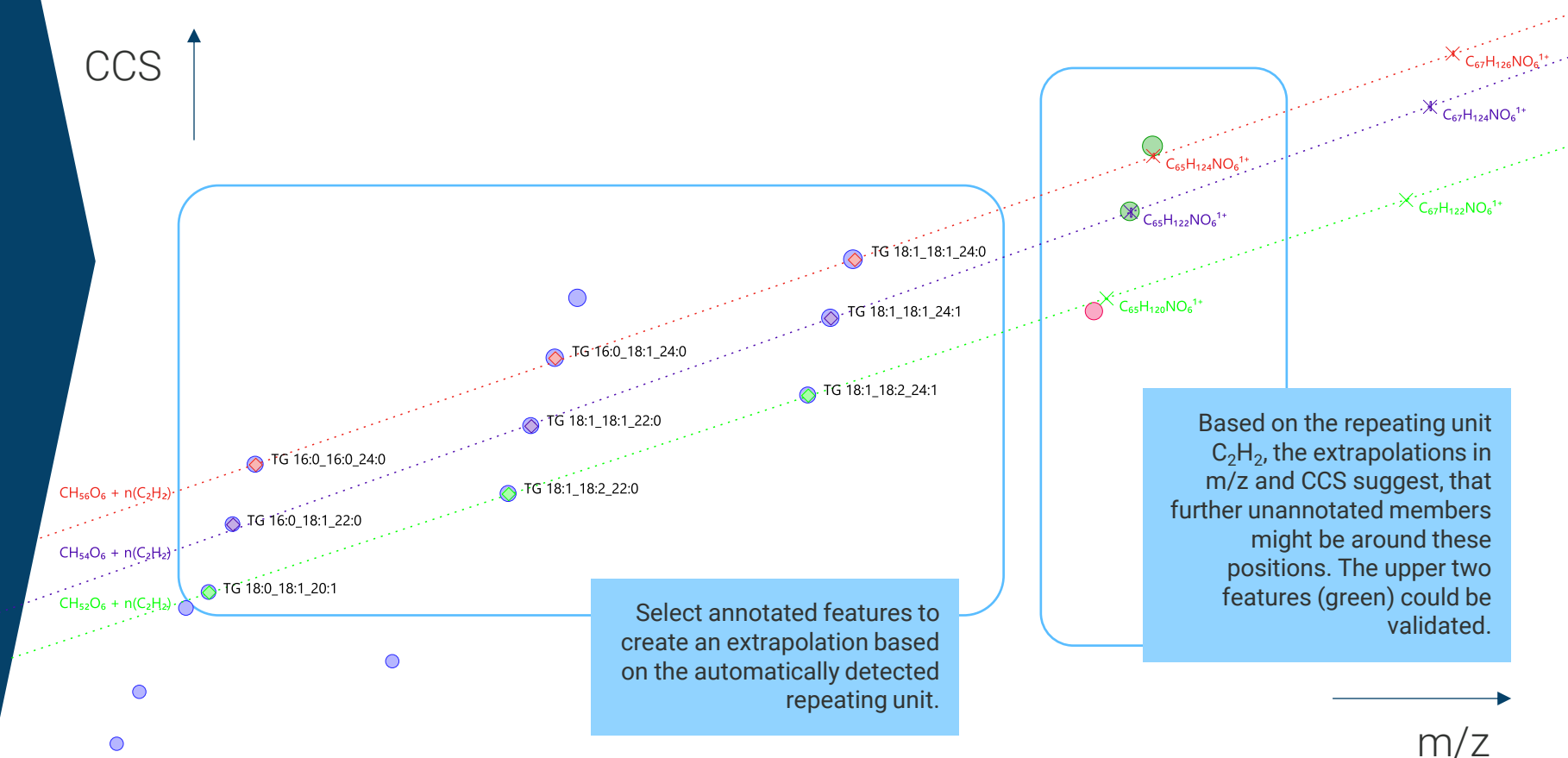


(Label options)

CCS [Å²]
 ● max: 348.8
 ○ min: 301.4

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

Metabolite Structure:

TL Succinic acid_2-3-NPH-Carbonyl-Carb TL Succinic acid_2-3-NPH-Carbonyl-Carb

Succinic acid_2-3-NPH-Carbonyl-Carboxy-Phospho
C₁₈H₁₈N₆O₈

Create TASQ method

Method Name
New TASQ method name

Derivatization and Fluxomics

MS/MS peak selection strategy (is not applied for Lipid Species annotations)

Select most intense peaks Select characteristic peaks

Number of most intense peaks
5

Ion selection strategy

Only Main Ion peaks

Fluxomics

Create isotopologues

Tracer isotope ¹³C ²H ¹⁵N ¹³C/²H ¹³C/¹⁵N

Create all isotopologues
 Create isotopologues in range A+ (min) to A+ (max)

Instrument Profile
 TOF TQ timsTOF

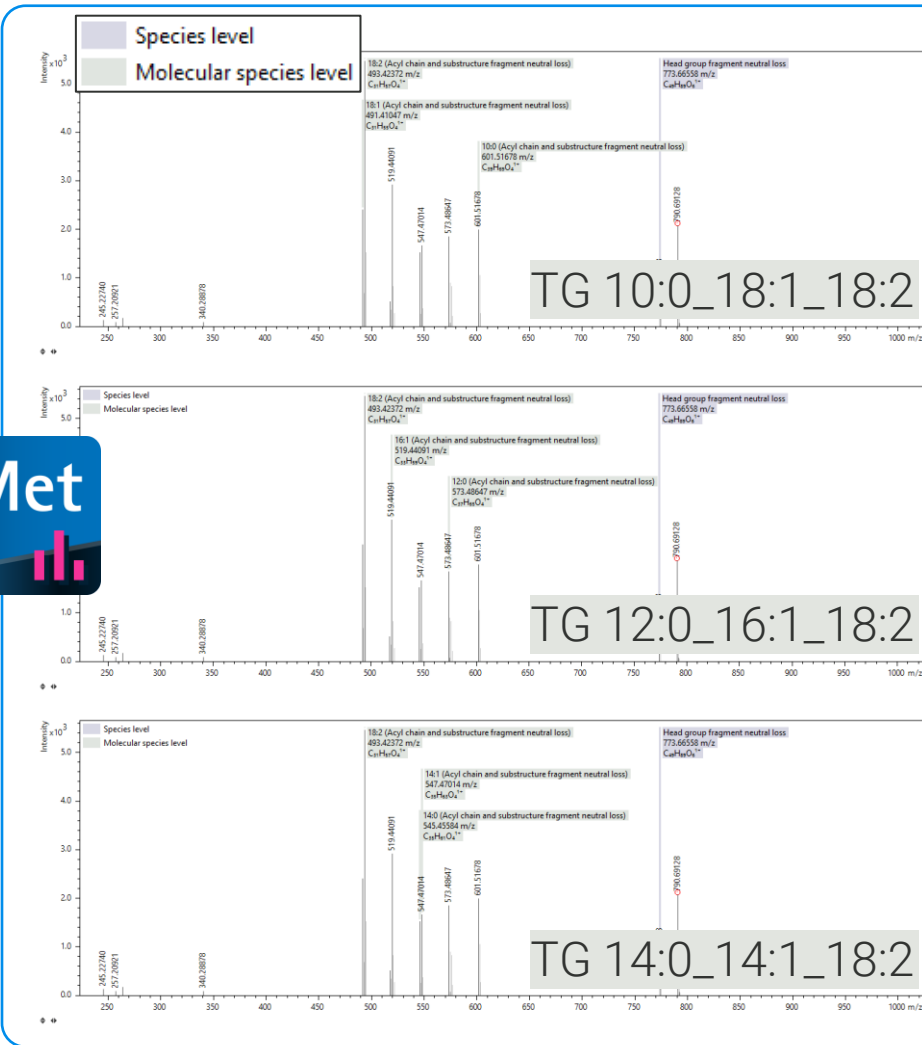
[timsTOF series negative]

Number of Features for TASQ Met

Create TASQ Fluxomics methods from within MetaboScape. Create ¹³C or other isotopologues based on the respective ¹²C 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.

	Ion	Ion formula	m/z	Spectrum type	Mandatory	Quant. ion
1	A+0	¹² C ₄ H ₆ ClO ₄ ¹⁻	152.9960	FullScan	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
2	A+1	¹² C ₃ ¹³ C ₁ H ₆ ClO ₄ ¹⁻	153.9994	FullScan	<input type="checkbox"/>	<input type="checkbox"/>
3	A+2	¹² C ₂ ¹³ C ₂ H ₆ ClO ₄ ¹⁻	155.0027	FullScan	<input type="checkbox"/>	<input type="checkbox"/>
4	A+3	¹² C ¹³ C ₃ H ₆ ClO ₄ ¹⁻	156.0061	FullScan	<input type="checkbox"/>	<input type="checkbox"/>
5	A+4	¹³ C ₄ H ₆ ClO ₄ ¹⁻	157.0094	FullScan	<input type="checkbox"/>	<input type="checkbox"/>

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
 $C_{31}H_{55}O_4^{1+}$

Create TASQ Method

Create TASQ method

Create TASQ method

Method Name

New TASQ method name

Lipidomics Method

MS/MS peak selection strategy (is only applied for Lipid Species annotations)

Respect all Lipid Species annotations of a Feature for MS/MS peak selection

Ion selection strategy

Only Main Ion peaks

Fluxomics

Create isotopologues

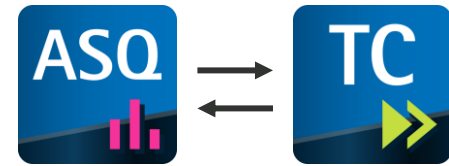
Instrument Profile

TOF TQ timsTOF

[timstof series positive]

Number of Features for TASQ Method: 12

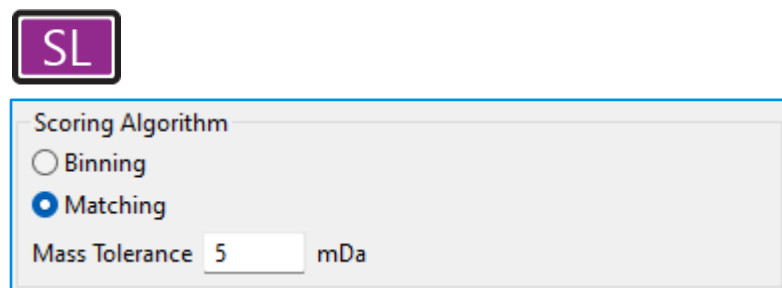
OK Cancel



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.

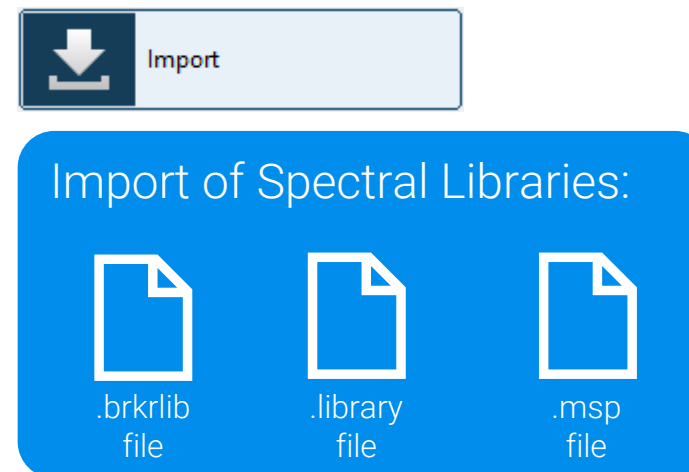
Spectral Library Improvements: Matching Algorithm and Import Performance

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



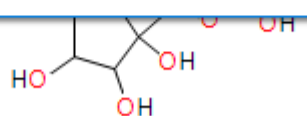
The import of the Spectral Library has been enhanced to run as a server task. This improvement not only boosts performance but, more importantly, ensures that the client user interface remains unblocked during the import.

Improved UI for *in-silico* derivatization methods

Target Molecule Test Structure

O=P(O)(O)OC[C@H]1O[C@](O)(COP(=O)(O)O)[C@@H](O)[C@@H]1O

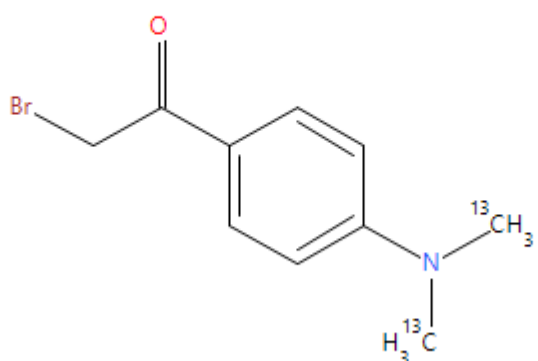
InChI=1S/C10H12N2O/c11-4-3-7-6-12-10-2-1-8(13)5-9(7)10/h1-2,5-6,12-13H,3-4,11H2
CC(C)C(CCCN(C)CCC1=CC(=C(C=C1)OC)OC)(C#N)C2=CC(=C(C=C2)OC)OC
CN(C)C1=CC=CC2=C1C=CC=C2S(=O)(=O)Cl
O=P(O)(O)OC[C@H]1O[C@](O)(COP(=O)(O)O)[C@@H](O)[C@@H]1O
CC(=O)C(=O)O



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.

Reagent Structure

[13CH3]N([13CH3])c1ccc(cc1)C(=O)CBr



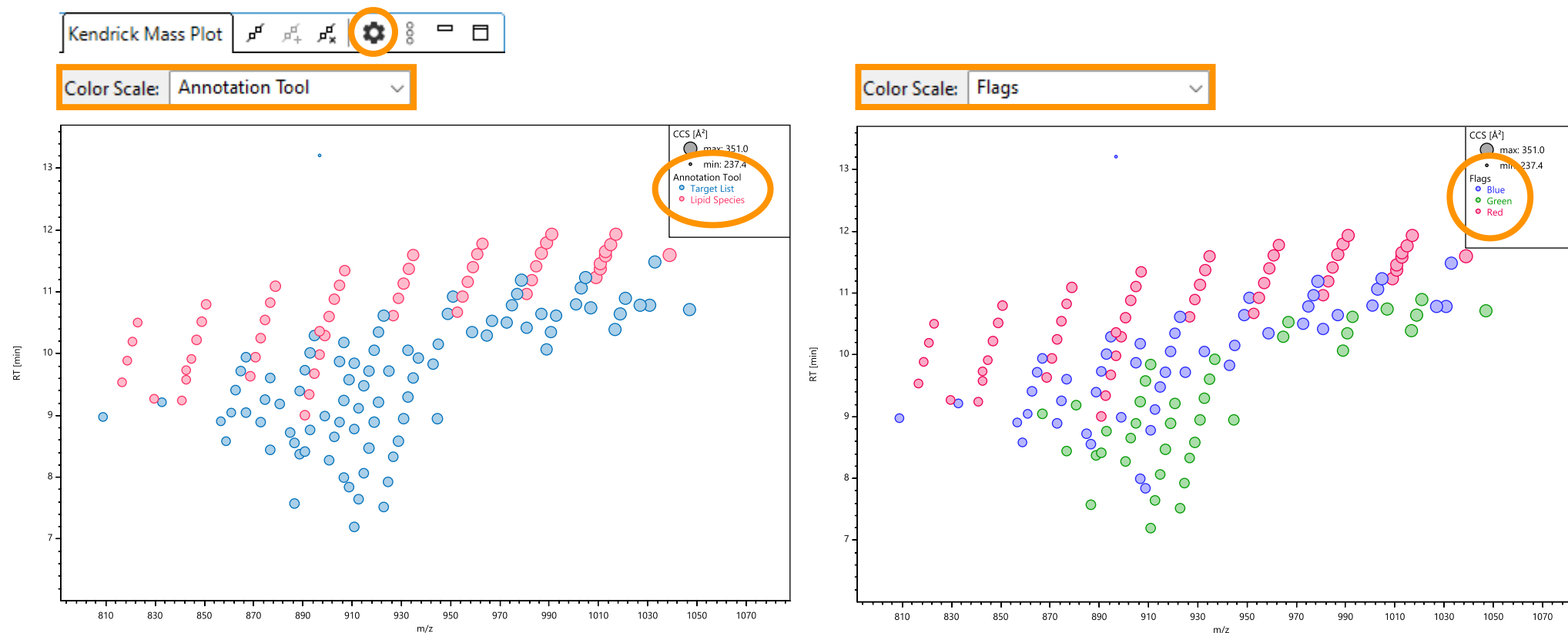
The *in-silico* derivatization user interface now also allows to validate methods designed for use with isotopically labelled derivatization reagents. Here, DmpA with two ¹³C atoms is used. In MetaboScape 2025b, isotopically labelled compounds require to turn off MetFrag *in-silico* fragmentation.



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

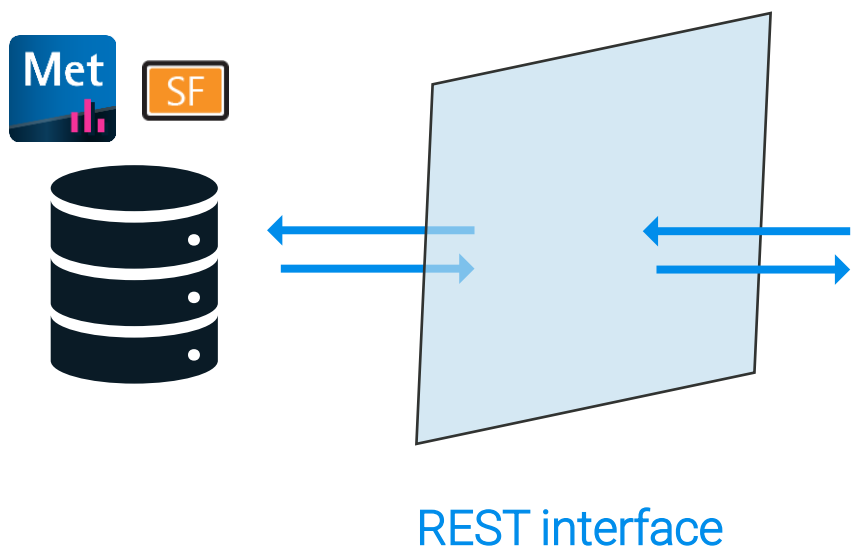


The new Color Scale options in the Kendrick Mass Plot / Survey View enable users to highlight features based on the annotation tools used or their first flag color. In the examples above, the left image shows TG lipids annotated with the **Lipid Species** tool, while further oxidized TGs were identified 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

MetaboScape server



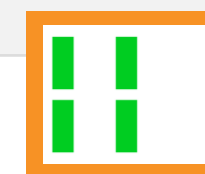
Apply MetaboScape's SmartFormula, including its metabolomics-tailored rule sets, within your own bioinformatics pipelines.

Your code:

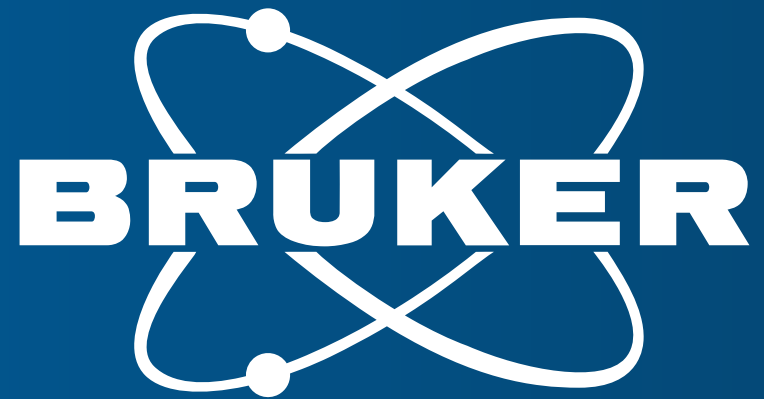
```
annotations = metaboscape_api.create_smartformula_annotations_with_method
```

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

Features



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



Innovation with Integrity