What’s new in MetaboScape® 2026b

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

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Cross Analyses MS/MS Comparison

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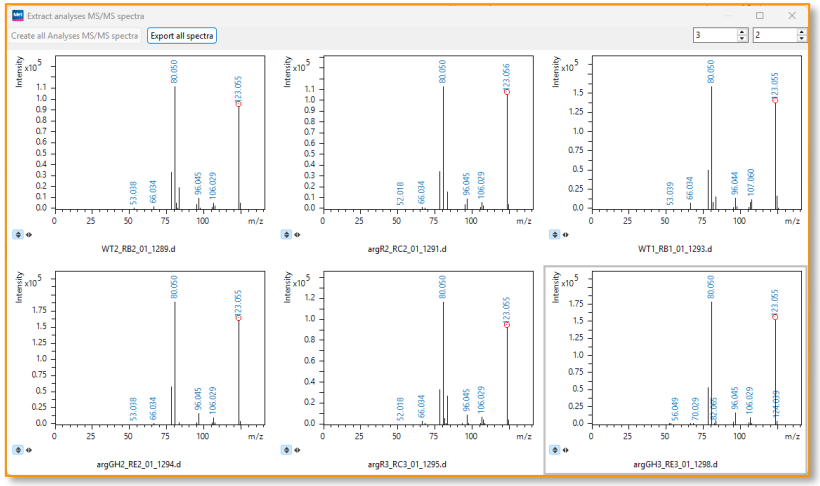
Find Isomer Heterogeneity

Cross Analyses MS/MS Comparison

DIGITAL METABOLOME ARCHIVE

Build your **Digital Metabolome Archive** and unlock it with MetaboScape

Access MS/MS spectra across all analyses of your Feature Table and **uncover differences in isomer composition** between sample groups.



Group A		*Group B*		*Group C*	
WT2_RB2_01_12...	WT1_RB1_01_1293.d	argGH3_RE3_01_12...	argGH2_RE2_01_12...	argR2_RC2_01_129...	argR3_RC3_01_129...
2435070	2435070	2435070	2435070	2435070	2435070
2329450	2432906	2423396	2435070	1366624	1600350
1811376	2073202	1315474	1432866	1575346	1570536

- Representative MS/MS spectrum from most intense precursor
- Additional MS/MS spectra, loaded on demand
- MS/MS spectra that exist, but have not yet been loaded
- These Features have not been picked as precursors for MS/MS acquisition

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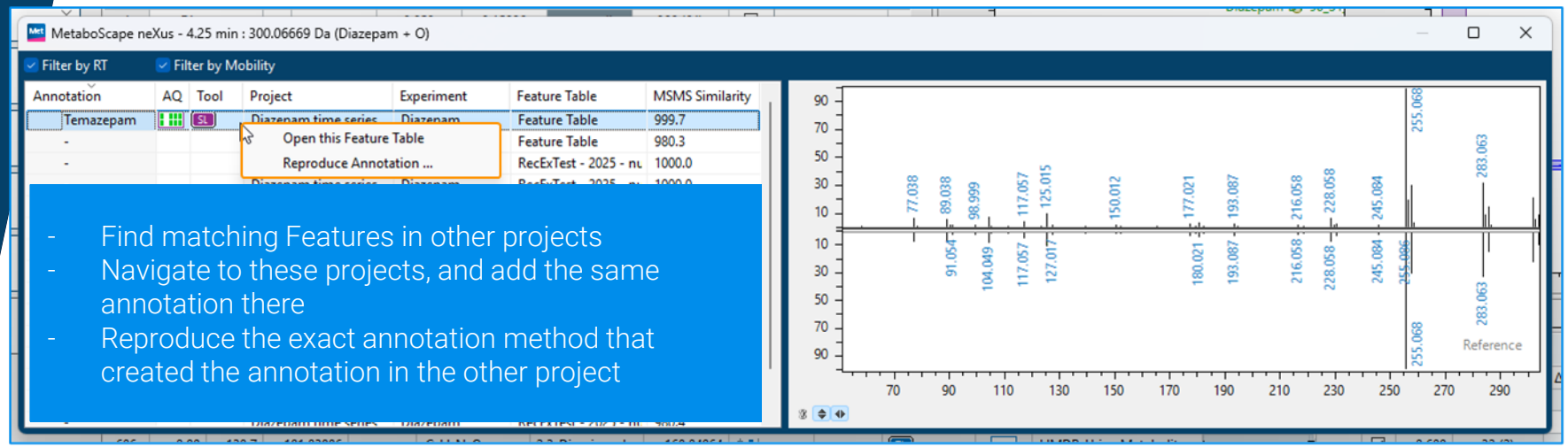
MetaboScape neXus

Cross Project Feature Matching

DIGITAL METABOLOME ARCHIVE

Build your **Digital Metabolome Archive** and unlock it with MetaboScape

By connecting projects across time, MetaboScape lets you see whether a feature or compound has appeared before, reuse validated annotations, and retrospectively enrich past experiments as new knowledge emerges.



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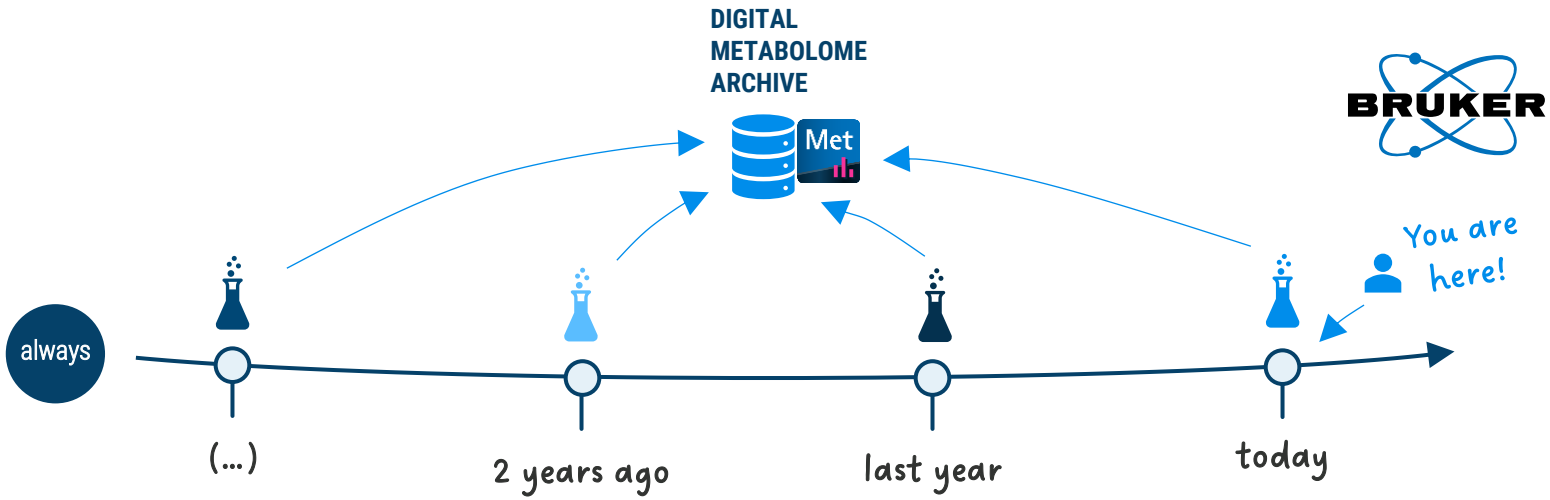
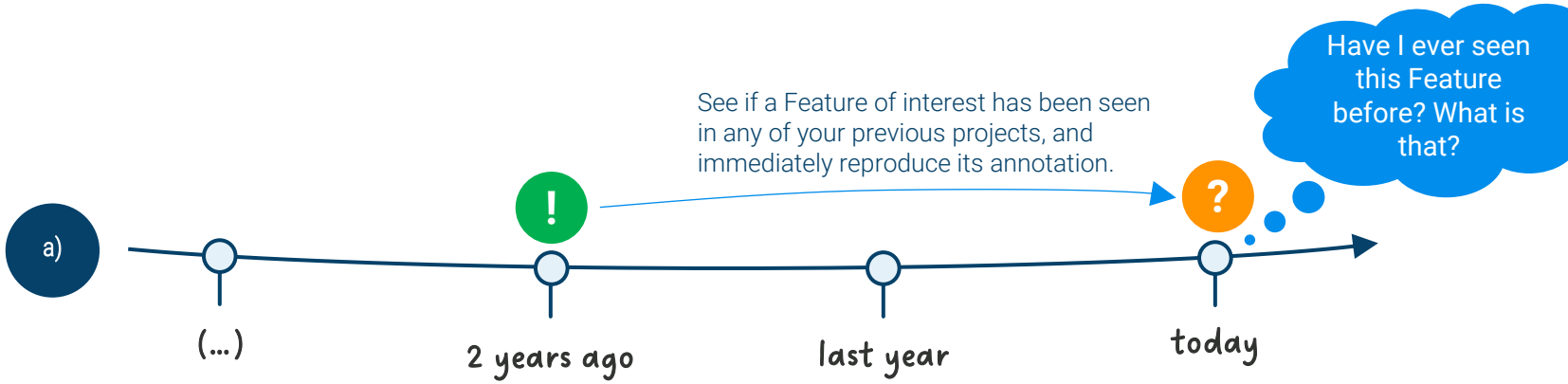
MetaboScape neXus

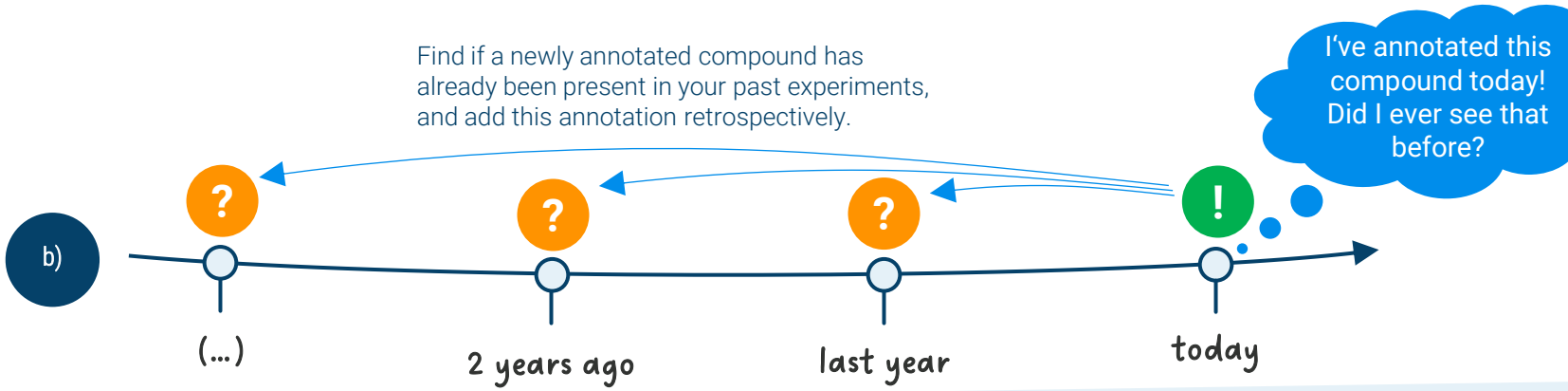
With MetaboScape's client-/server-architecture, all the projects, feature tables and annotations that you create over the years, are stored in the same database.



A certain Feature of interest may have been found and annotated in a previous project already. Find these Features, see how they were annotated, and eventually reproduce the same annotation in your current project.



A compound that can be annotated just today, may have been present in experiments in the past. Find out in which previous projects that compound has occured, but could not be annotated at that time.



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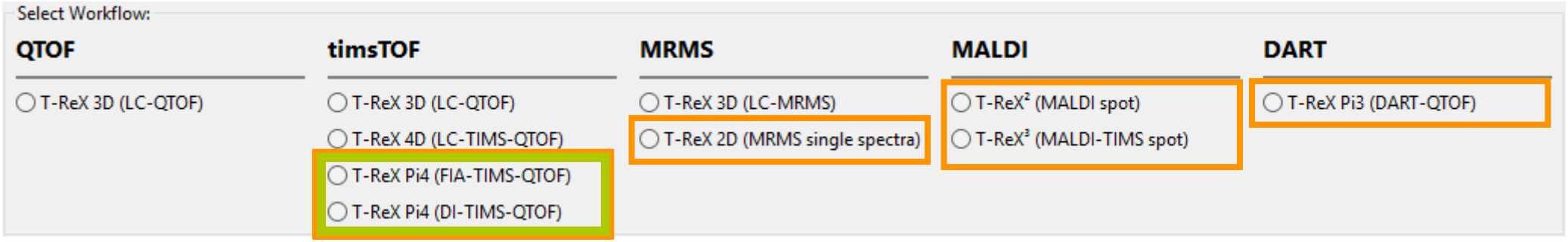
FIA- and DI-TIMS data processing with T-ReX Pi4



Chromatography free workflows

Newly added in 2026b

T-ReX Pi3 and Pi4 are applicable to raw data that has a time dimension, but no retention time. In different ways, this data is projected (typically denoted with π (pi)) and then further processed as chromatography-free data.

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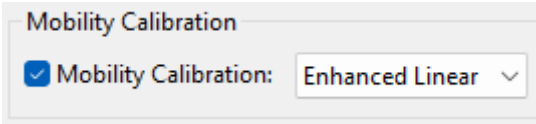
Enhanced Linear Mobility Calibration

Compass for timsTOF series 2026b



Supporting

- Reading data with enhanced linear instrument calibration
- Recalibration of data with enhanced linear calibration

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Custom Rule-based Annotation for systematically defined compound classes

Human-readable configuration file format

- Use MetaboScape's new custom rule-based annotation system for compound classes of your interest.
- Built to systematically expand homologous series in multiple dimensions.

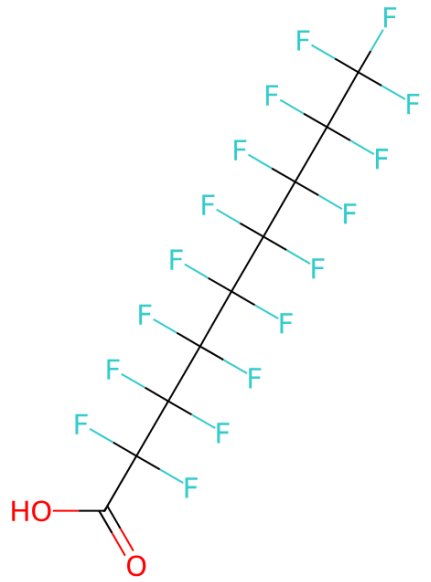
Exemplified and Validated

The custom rule-based annotation system could already be applied across diverse lipid classes (incl. Isoprenoid groups and rings) and PFAS.

AppNotes available

See the Literature Room at bruker.com/metaboscape

- LCMS 252
  GPNAE HOMOLOGOUS ROWS
- MSI 47
  RULE-BASED ANNOTATION

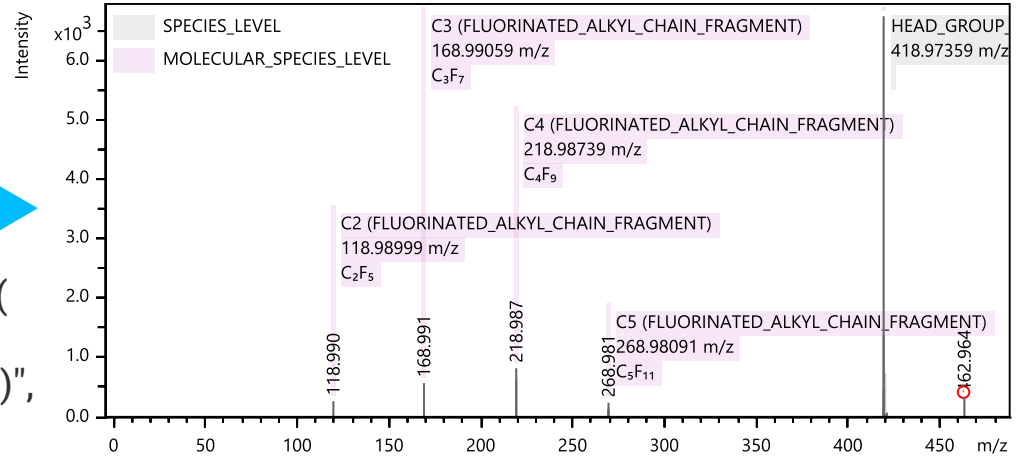


annotationName: "C{numberOfCarbons}-PFCA"

label: "FLUORINATED_ALKYL_CHAIN_FRAGMENT",

query: "QUERY scaninfo(MS2DATA) WHERE MS2PROD=formula(
C{numberOfCarbonsPerFragment}
+F({numberOfCarbonsPerFragment}*2+1))",

C8-PFCA



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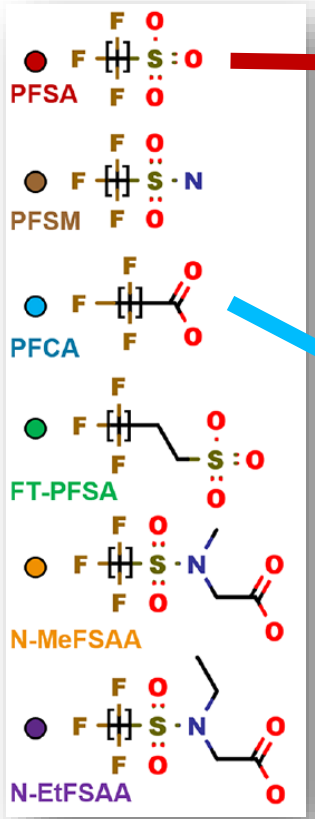
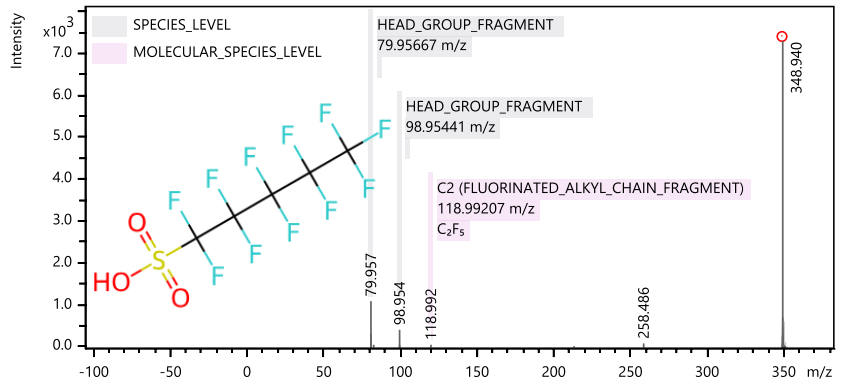
Custom Rule-based Annotation for systematically defined compound classes – Example: Homologous Series of PFAS

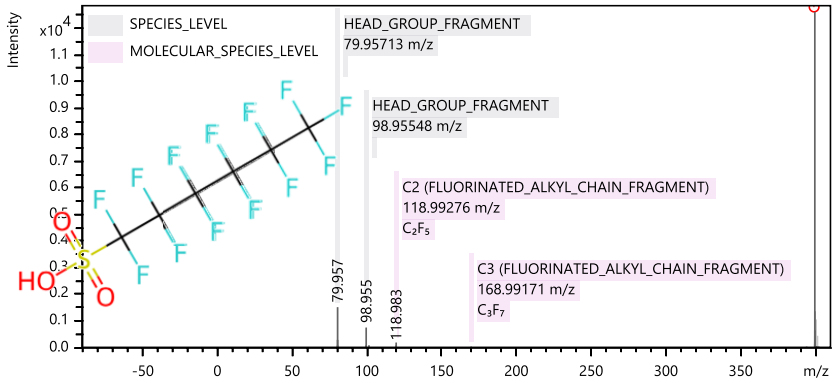


Koelmel *et al.*, ACS, 2020

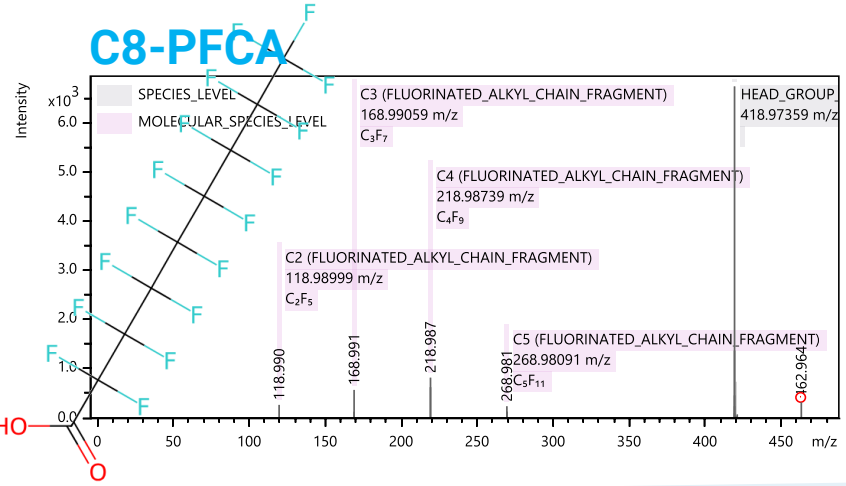
C5-PFSA



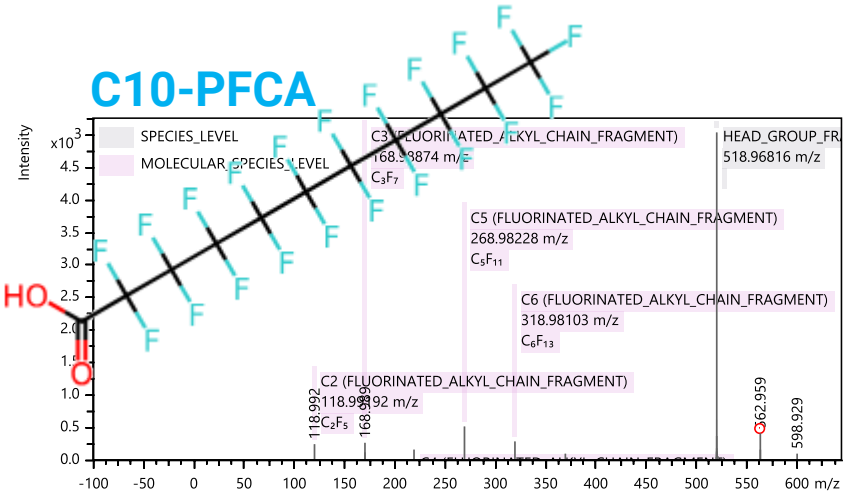
C6-PFSA



C8-PFCA



C10-PFCA



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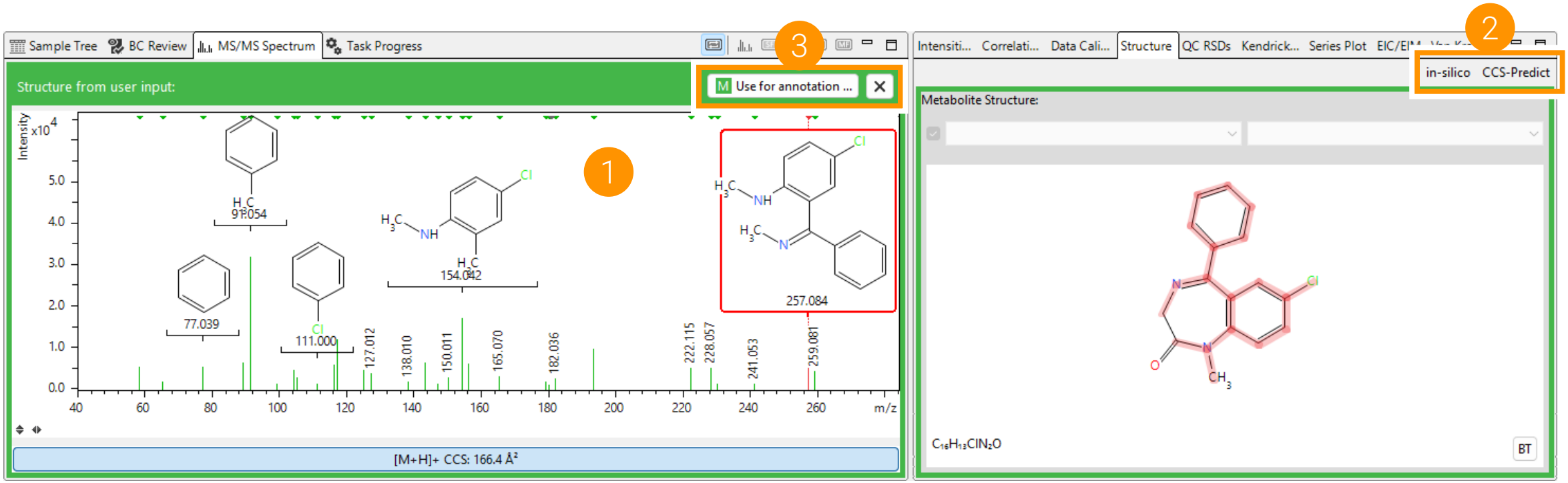
Ad-hoc Structure Verification

Copy and paste (Ctrl+c, Ctrl+v) SMILES or InChI structures directly into the **MS/MS Spectrum** 1 view to instantly evaluate their match with **MetFrag** *in-silico* fragmentation and **CCS-Predict** 2 . Apply the structure for annotation or simply dismiss the temporary result with a single click 3 .

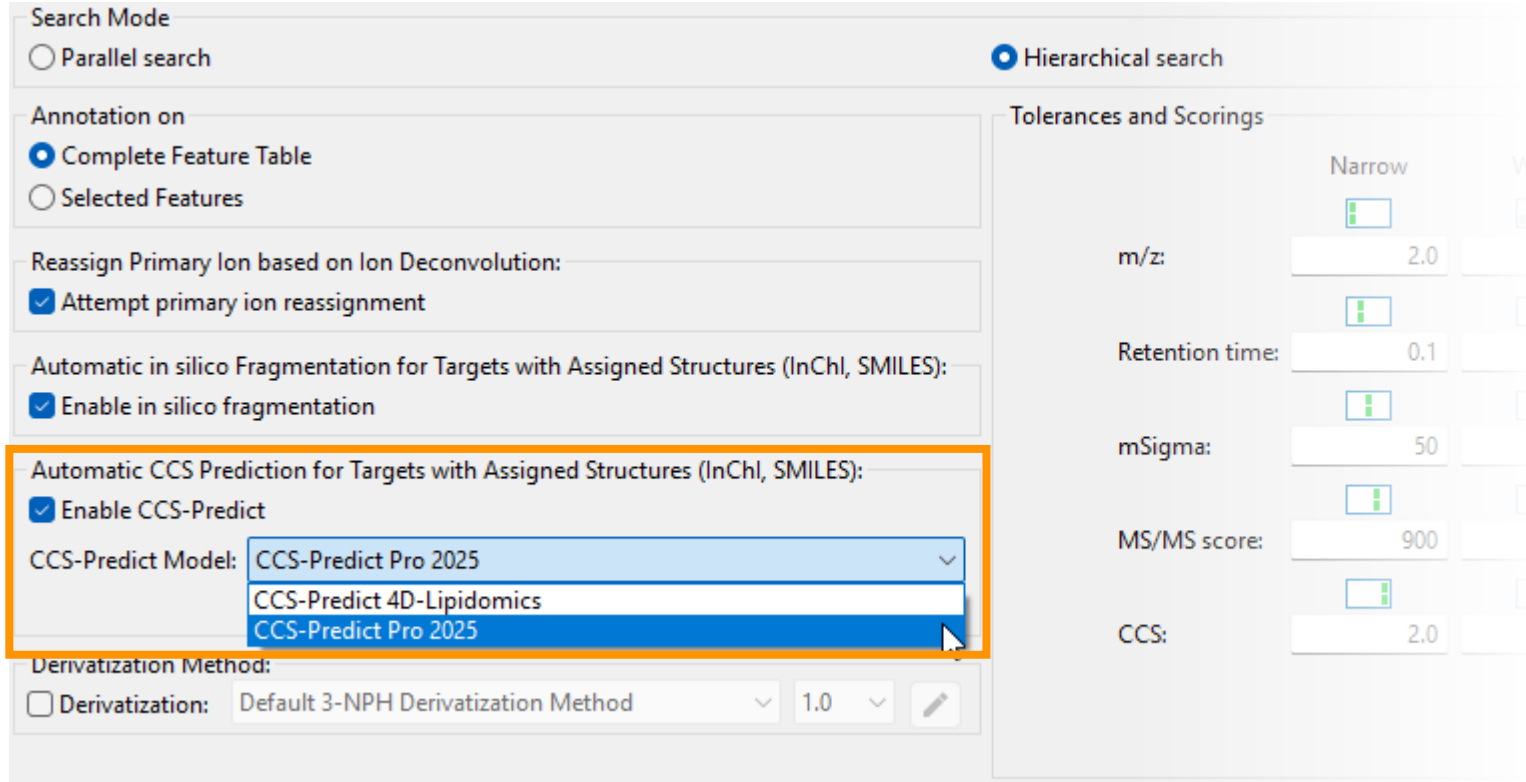


Select CCS-Predict Models for Automated Annotations

TL SL CCS-Predict

For both, automated annotation with Target List or Spectral Library, choose which CCS prediction model you want to apply.
In the current version, two models are available:

- CCS-Predict 4D-Lipidomics
- CCS-Predict Pro 2025



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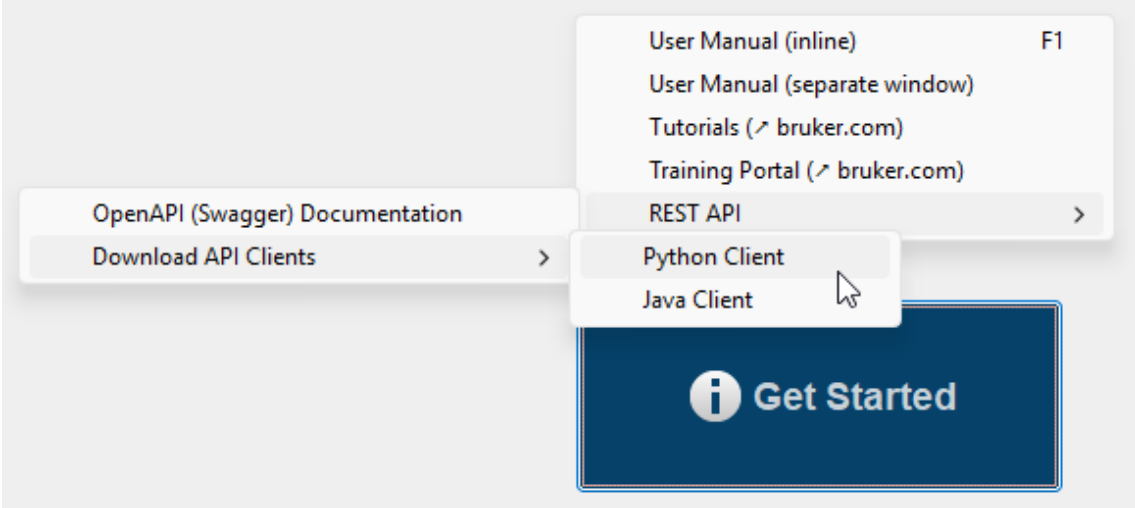
REST-API Updates

API Changes

- Added **creationDate** to **Project**, **Experiment** and **FeatureTable**
- Added **description** to **Project** and **Experiment**
- Added **SampleVolume** to **Sample**
- Added **FilePathInfo** with **stationName** and **path** to **Analysis**

Download compatible Python or Java clients

- Added download links to Python and Java clients, compatible to the current server, to the Get Started button the Home perspective.



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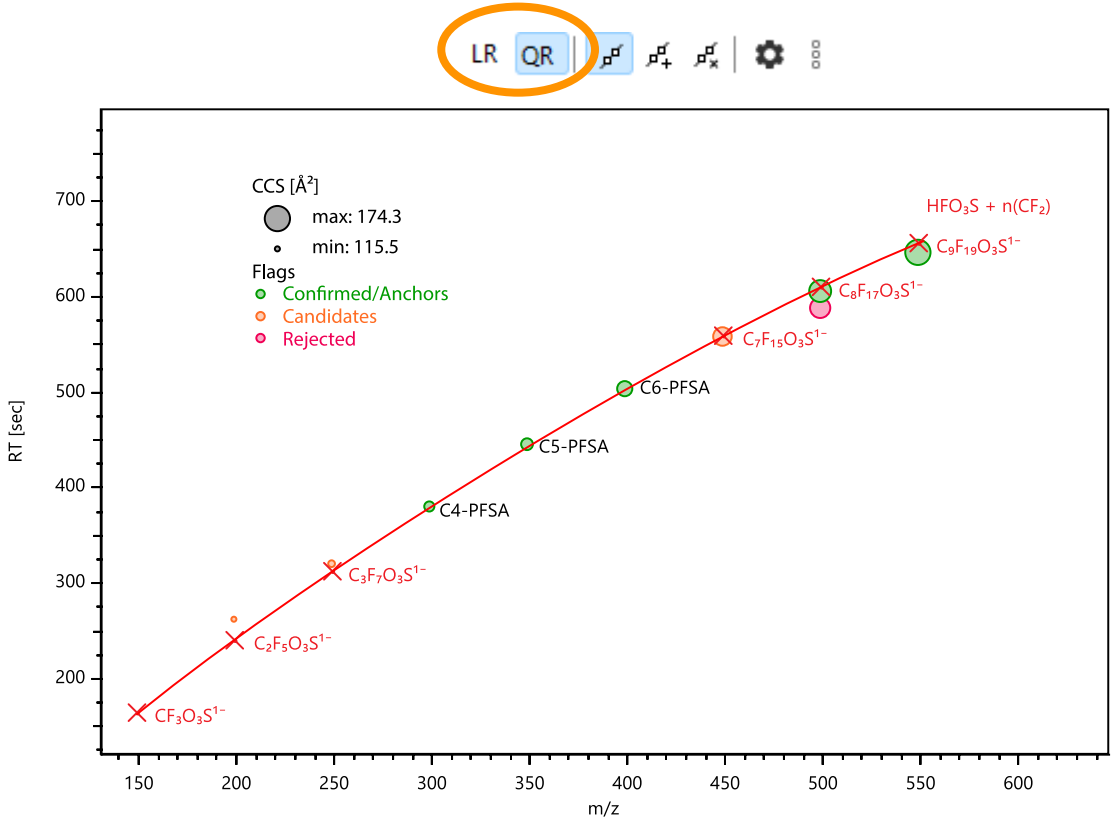
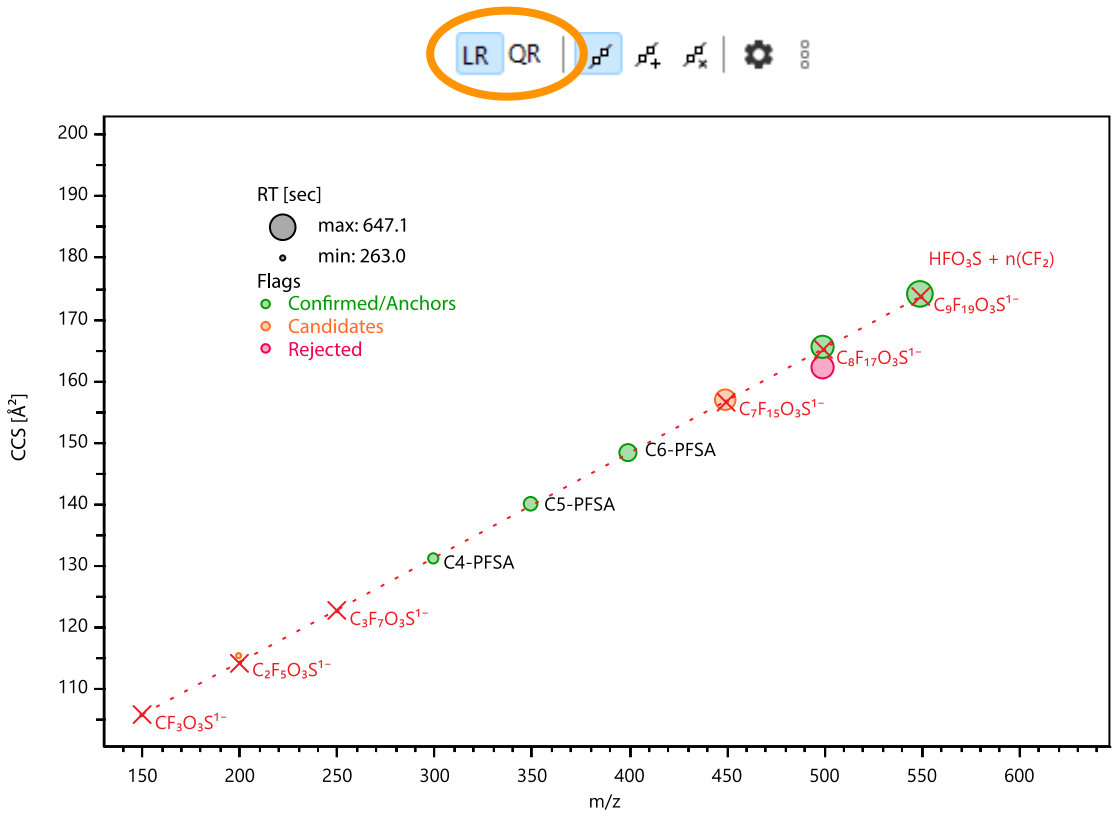
Quadratic Homologous Series Extrapolation

The Homologous Series Extension tool has been enhanced with support for quadratic regression and extrapolation. Once you have selected anchor features and generated a series, you can toggle linear or quadratic regression using the LR and QR buttons.





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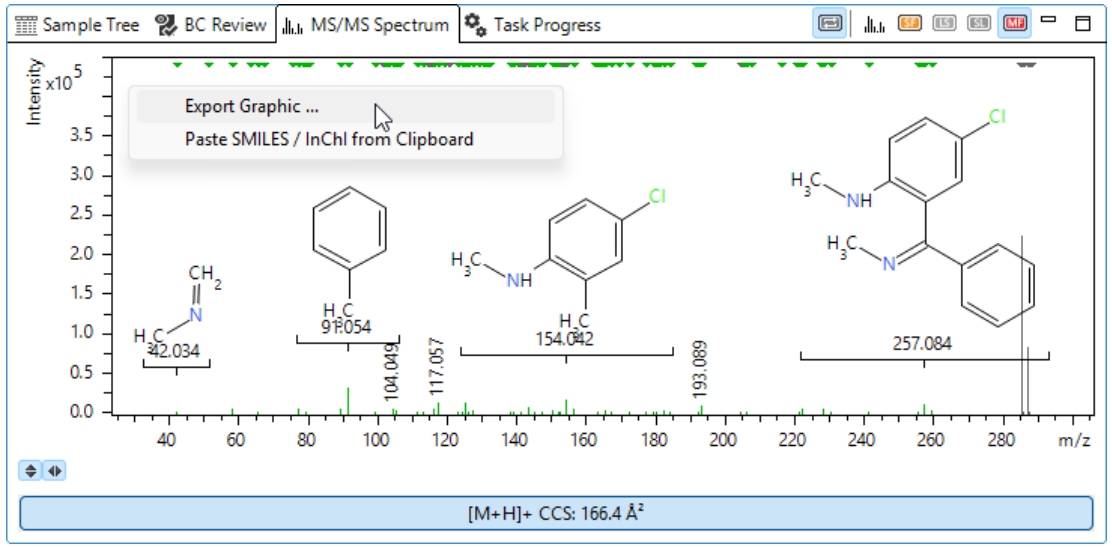
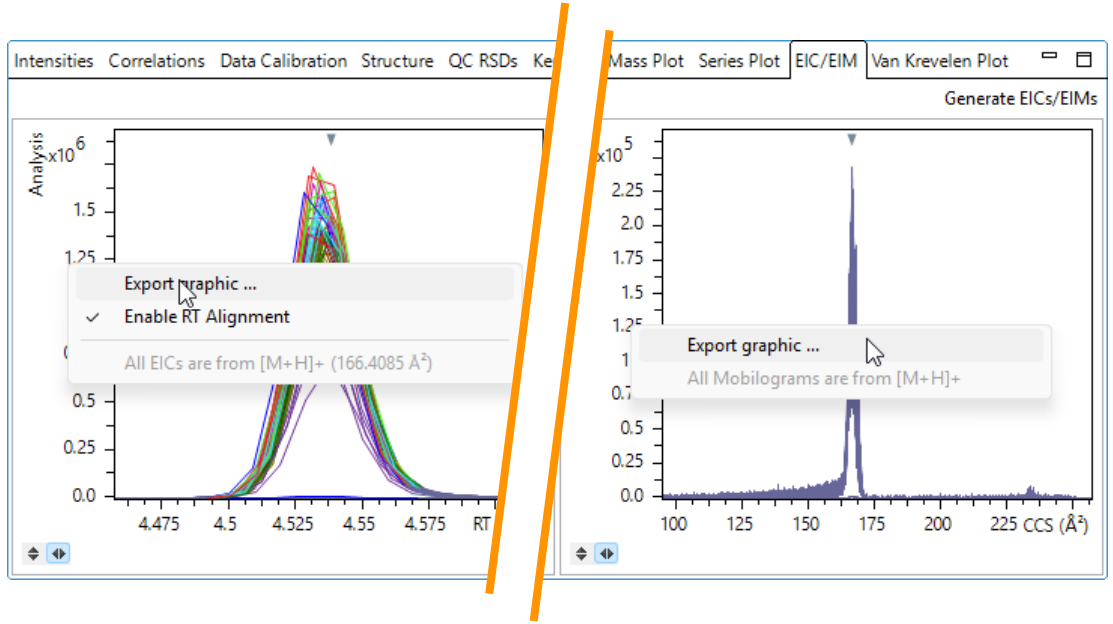
Export of MS/MS, EIC, and EIM images

Export all flavours of the MS/MS Spectrum view as well as EICs and EIMs as .svg, .png, .gif, or .emf file.





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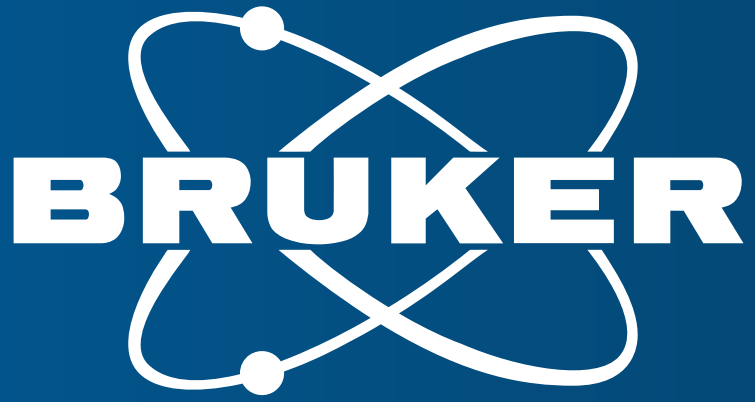

Innovation with Integrity