

TASQ 2026

# TASQ 2026 What is new?

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# TASQ 2026

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- Support timsMetabo in TASQ QSee Performance Test Tool
- Support GC-TQ – Basic data processing and quantification available
- Support GC and UV data only – add instrument type **Other**
- Support internal performance standard for EPA 533 and 1633

## TASQ 2026: Minor Features

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- Show Compound Heat Map
  - Show heat maps for each ion in all three major faces
  - Swap x-y axis and arrange the three faces by drag and drop for better comparison
  - Overlay method information and actually used ranges
- Check TASQ processing methods for errors
  - Do not start processing if method will potentially inconsistent or wrong results
  - Indicate what needs to be changed to fix the method
- Do not allow import of batches if Bruker MS Data Processing is not available, required for reading meta data from data sets

## TASQ 2026: Minor Features

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- Improvements Analyte Navigator
  - Sort analytes by RT or name
  - Tree view Analytes vs Internal Standards and Internal Performance Standard
- Multi Chromatograms/Mobilograms view: show traces of internal standards when data source Determination is selected
- Chromatogram(s)/Mobilogram(s) view – new option show traces of quantifier ions only
- Chromatogram/Mobilogram view: overlay intensity threshold of peak finder for chromatogram of principle ion
- Specify chromatogram peak finder mode on ion level (Classic, Valley to Valley, EMG)
- List Chromatogram view – remember settings and restore them after client restart

## TASQ 2026: Minor Features

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- Set user flags in result tables by key shortcuts CTRL+SHIFT+U, 0-6 or CTRL+SHIFT+U, c <- clear flag or 0
- Set review state in result tables by key shortcuts CTRL+SHIFT+R, 0-5
- Update Parameters Wizard: choose version of method which shall be updated
- Improvements SmartFormula view: add to TASQ method: edit spectrum type
- Batch Statistics graph: swap x and y attribute types directly with a swap button
  - Overlay cumulative probability curve if rank is the chosen attribute. A normal distribution of the other attribute is assumed using the mean and standard deviation of the other attribute to calculate the cumulative probability curve
  - Overlay guidelines mean +/- standard deviation
  - Added option to show data points only for found determinations

## TASQ 2026: Minor Features

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- Improved error notification in method editor
- Method editor -> Rule False Negative can't be deselected anymore
- Exchange of analyte method parameters by tsv text file extended
- Improved detection of inconsistent settings of RT ranges when Peak Group is selected for integration
- Batch Setup Wizard can handle new TQ workflow methods

## TASQ 2026: Audit Trail extended

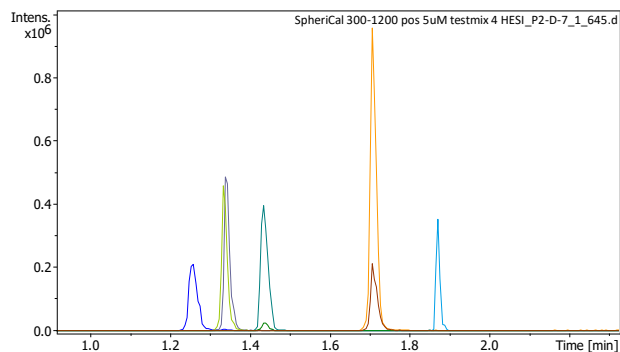
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- Currently TASQ 2026 is not usable for regulated applications
- Added audit trail for command „Library Search on Determination“

# Introduction of QSee™ products

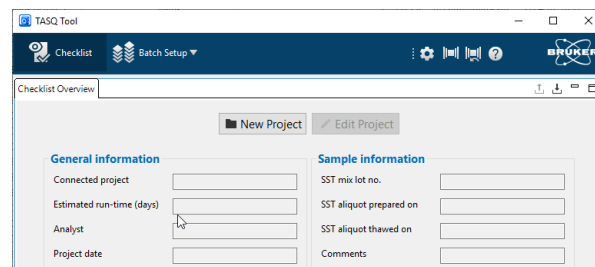
## Reference Standard Mixture

### QSee 8-Mix



## Software

### QSee Performance Test Software



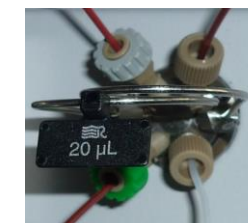
Featuring



1290 Infinity II



VIP-HESI source



6-port valve



timsMetabo



timsTOF HT



timsTOF Pro 2

# QSee Performance Testing – Overview on the Workflow

Collection of QC related system information

Starting data acquisition & automatic reporting with very few clicks

**QSee**  
Performance Test SW

Automatic upload of data to TwinScape (GUI may differ)

TASQ-based batch reporting (screenshots may differ from QSee report)

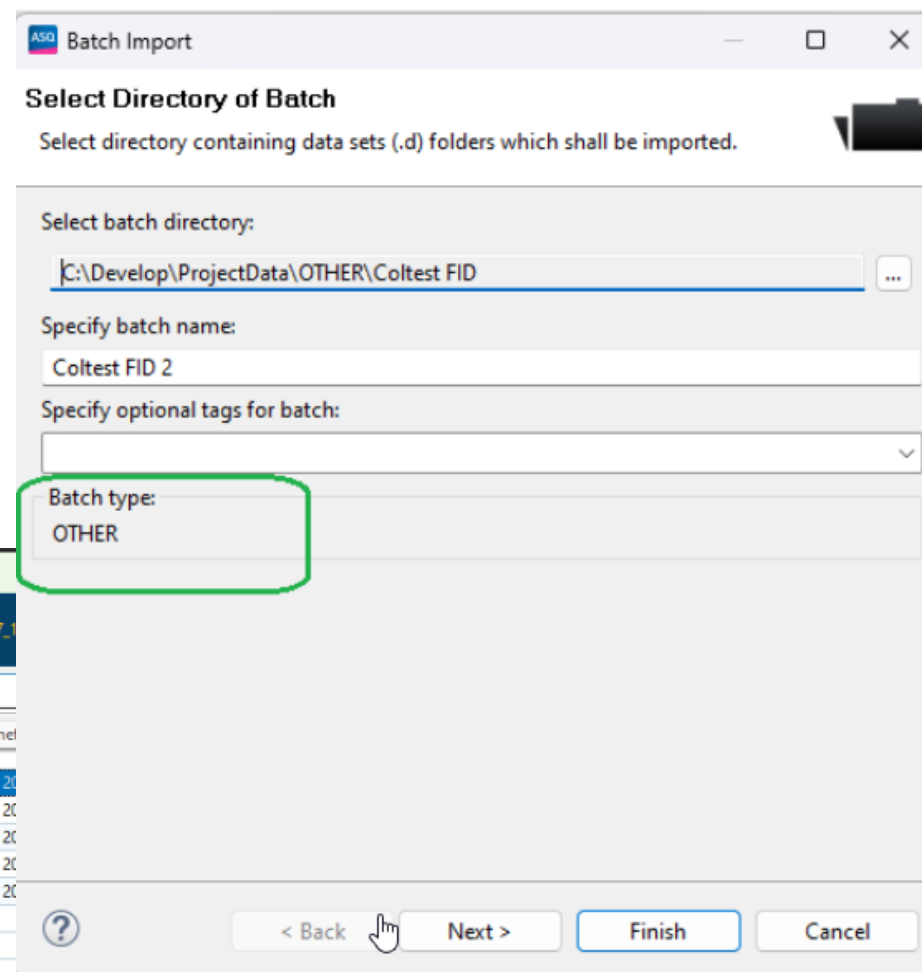
## TASQ 2026: Support for GC data processing

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- Introduced instrument type Other for GC and UV data only without MS data
- Enabled import of GC or UV data only batches without MS data
- Enhance TASQ method to handle and create GC traces
- Enhance TASQ method to specify retention time offsets for GC detections in front, middle and rear position
- Implemented processing of GC traces
  - Load traces from chromatography-data.sqlite
  - Process traces like UV traces – smooth – peak detection
  - Store GC findings

# TASQ 2026: New Instrument Type: Other – GC and UV data only

- Support batches with data like UV and GC but no MS data
  - New instrument type Other



ASQ Batch Import

Select Directory of Batch

Select directory containing data sets (.d) folders which shall be imported.

Select batch directory:

C:\Develop\ProjectData\OTHER\Coltest FID

Specify batch name:

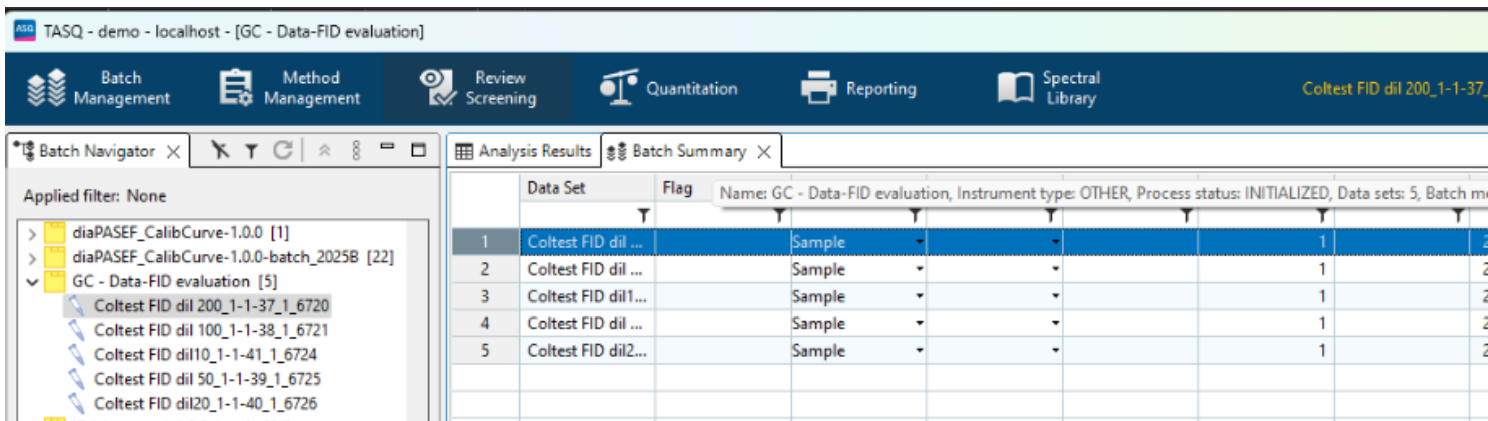
Coltest FID 2

Specify optional tags for batch:

Batch type:

OTHER

< Back Next > Finish Cancel



TASQ - demo - localhost - [GC - Data-FID evaluation]

Batch Management Method Management Review Screening Quantitation Reporting Spectral Library Coltest FID dil 200\_1-1-37\_1

Batch Navigator x Batch Summary x

Applied filter: None

- diaPASEF\_CalibCurve-1.0.0 [1]
- diaPASEF\_CalibCurve-1.0.0-batch\_2025B [22]
- GC - Data-FID evaluation [5]
  - Coltest FID dil 200\_1-1-37\_1\_6720
  - Coltest FID dil 100\_1-1-38\_1\_6721
  - Coltest FID dil10\_1-1-41\_1\_6724
  - Coltest FID dil 50\_1-1-39\_1\_6725
  - Coltest FID dil20\_1-1-40\_1\_6726

Data Set	Flag	Name: GC - Data-FID evaluation, Instrument type: OTHER, Process status: INITIALIZED, Data sets: 5, Batch me
1	Coltest FID dil ...	Sample
2	Coltest FID dil ...	Sample
3	Coltest FID dil1...	Sample
4	Coltest FID dil ...	Sample
5	Coltest FID dil2...	Sample

# TASQ 2026: TASQ Method – General Settings – GC RT Offset

Detector Configuration

Detector type **GC**

GC Front RT offset 0.00 [s]

GC Middle RT offset 0.00 [s]

GC Rear RT offset 0.00 [s]

Detector Configuration

Detector type **UV**

UV-VIS RT offset 15.00 [s]

Method Editor x Method Matcher Method Profile Manager

Selected method: **UV IS (V2) 1 [Vers.: 9 / timsTOF]** Version: 9 (2025-03-28 10:21:54)

General method settings | timsTOF settings | Calibration settings | Analytes settings | Quantitation settings | Library search settings | General library search settings | Internal standards | Extracted internal standards | NI

Read-only method

Determination ion quality: Principal ion and at least one mandatory ion

Determination filter: Most mandatory and closest to RT

Chromatogram peak finder mode: Classic

Batch concentration levels: [ ] [ ] [ ]

Ion Ratio Signal Type: HEIGHT

Perform smoothing

Perform Denoising (not applied for timsON data)

Max/Min A/H upper limit: 0.000

Minimal datapoints over a peak: 10

Only create chromatogram slices of  $\pm$  0.75 [min]

Check here whether you want to create a short chromatogram within a specified time range.

narrow m/z window of ms spectra  $\sim$ -2+5 m/z

Signal / Noise Parameters

Algorithm: Classic

S/N filter: 5.000

Surrogate noise: 1.000

DART Parameters

Enable ChromatograFree processing

Time start: [ ] [min]

Time end: [ ] [min]

Detector Configuration

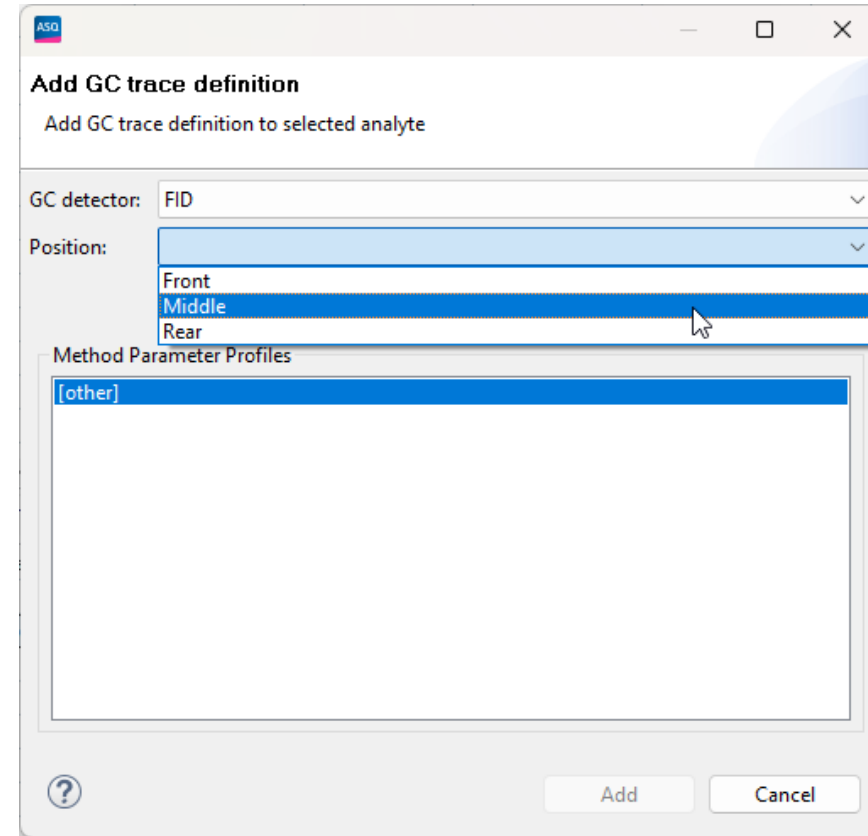
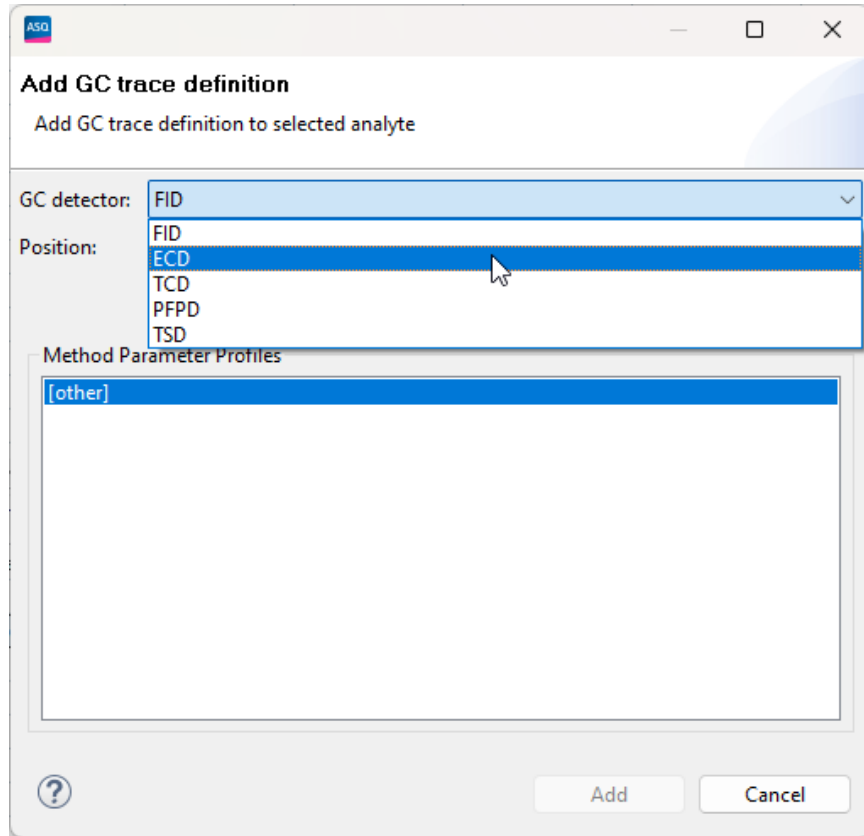
Detector type: **GC**

GC Front RT offset 12.00 [s]

GC Middle RT offset 0.00 [s]

GC Rear RT offset 0.00 [s]

# TASQ 2026: TASQ Method: GC – Trace Definitions



- Supported GC detectors: FID, ECD, TCD, PFDP, TSD

## TASQ 2026: TASQ Method Editor – GC Traces

- Trace definitions for GC in method editor
- Specify GC detector and detector position
- Specify whether a peak has to be detected (Mandatory) and used for quantification (Quantifier)

	Analyte	GC Detector	Detector Positi...	Mandatory	Quant. GC trace	Area thr.	Height thr.	Sens. [%]	Min peak valley [%]	Smoothing width t[s]
1	n-Nonanal	FID	Front	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1	2	99	4.0	1.00

# TASQ 2026: Result Columns for GC and UV Results

Area (GC) for Quantification  
 Height (GC) for Quantification  
 Rel. Area GC  
 Rel. Height GC  
 Rel. Quantity (GC Area)  
 Rel. Quantity (GC Height)

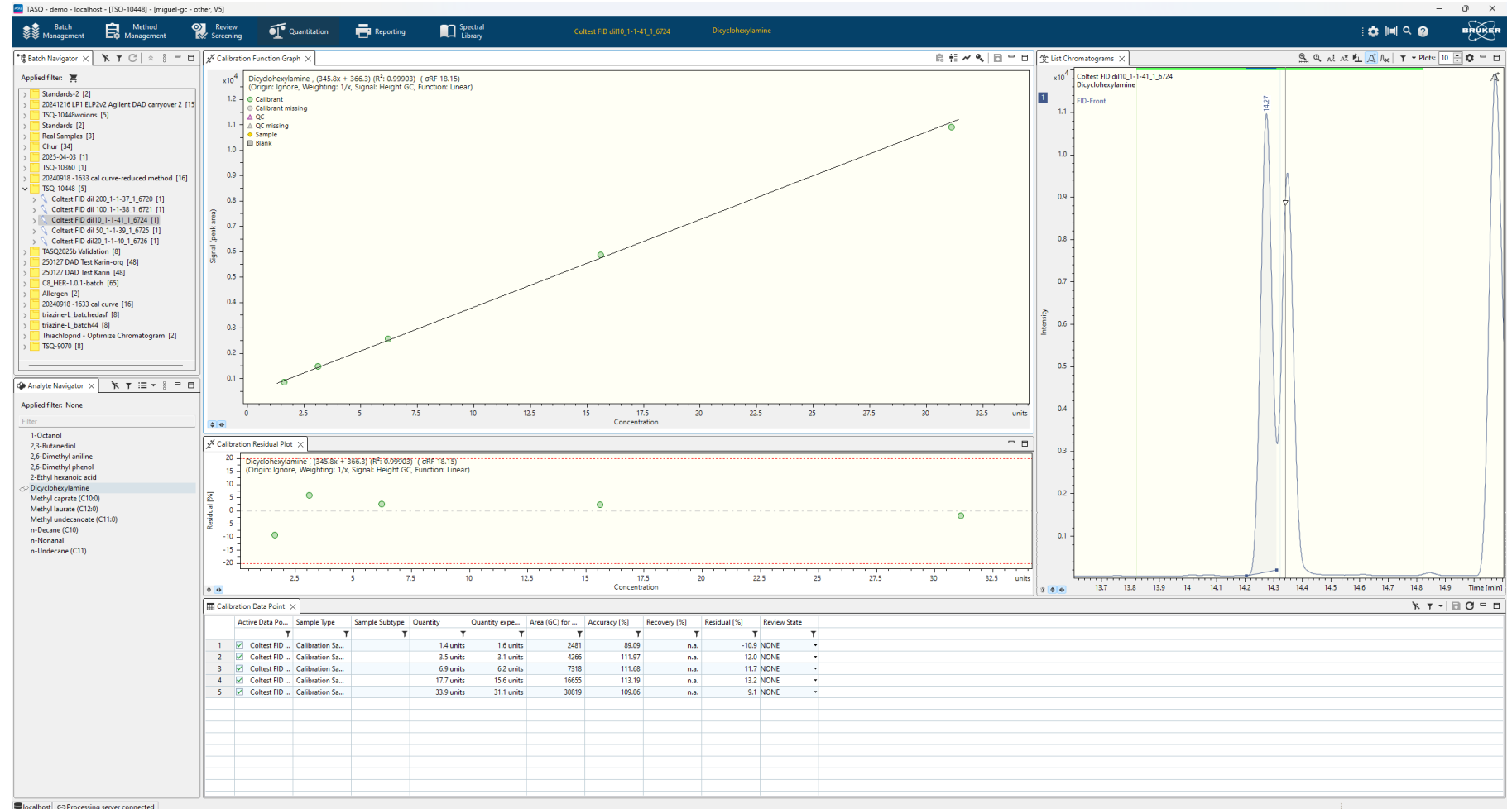
Sum of GC area values of all quantifier ions  
 Sum of GC height values of all quantifier ions  
 Area GC relative to internal standard  
 Height GC relative to internal standard  
 Relative quantity based on internal standard  $c = (\text{Signal Area for Quantification GC} / \text{Signal IS GC}) * c_{IS}$   
 Relative quantity based on internal standard  $c = (\text{Signal Height for Quantification GC} / \text{Signal IS Height GC}) * c_{IS}$

Area (UV-VIS) for Quantification  
 Area for Quantification [IS] (UV-VIS)  
 Area for Quantification [IPS] (UV-VIS)  
 Height (UV-VIS) for Quantification  
 Height for Quantification [IS] (UV-VIS)  
 Height for Quantification [IPS] (UV-VIS)  
 Rel. Area UV-VIS  
 Rel. Height UV-VIS  
 Rel. Quantity (UV-VIS Area)  
 Rel. Quantity (UV-VIS Height)

Sum of UV-VIS area values of all quantifier ions  
 Area of UV-VIS chromatogram peak for internal standard  
 Area of UV-VIS chromatogram peak for internal performance standard  
 Sum of UV-VIS height values of all quantifier ions  
 Height for Quantification [IS] (UV-VIS)  
 Height for Quantification [IPS] (UV-VIS)  
 Area UV-VIS relative to internal standard  
 Height UV-VIS relative to internal standard  
 Relative quantity based on internal standard  $c = (\text{Signal Area for Quantification UV-VIS} / \text{Signal IS UV-VIS}) * c_{IS}$   
 Relative quantity based on internal standard  $c = (\text{Signal Height for Quantification UV-VIS} / \text{Signal IS Height UV-VIS}) * c_{IS}$

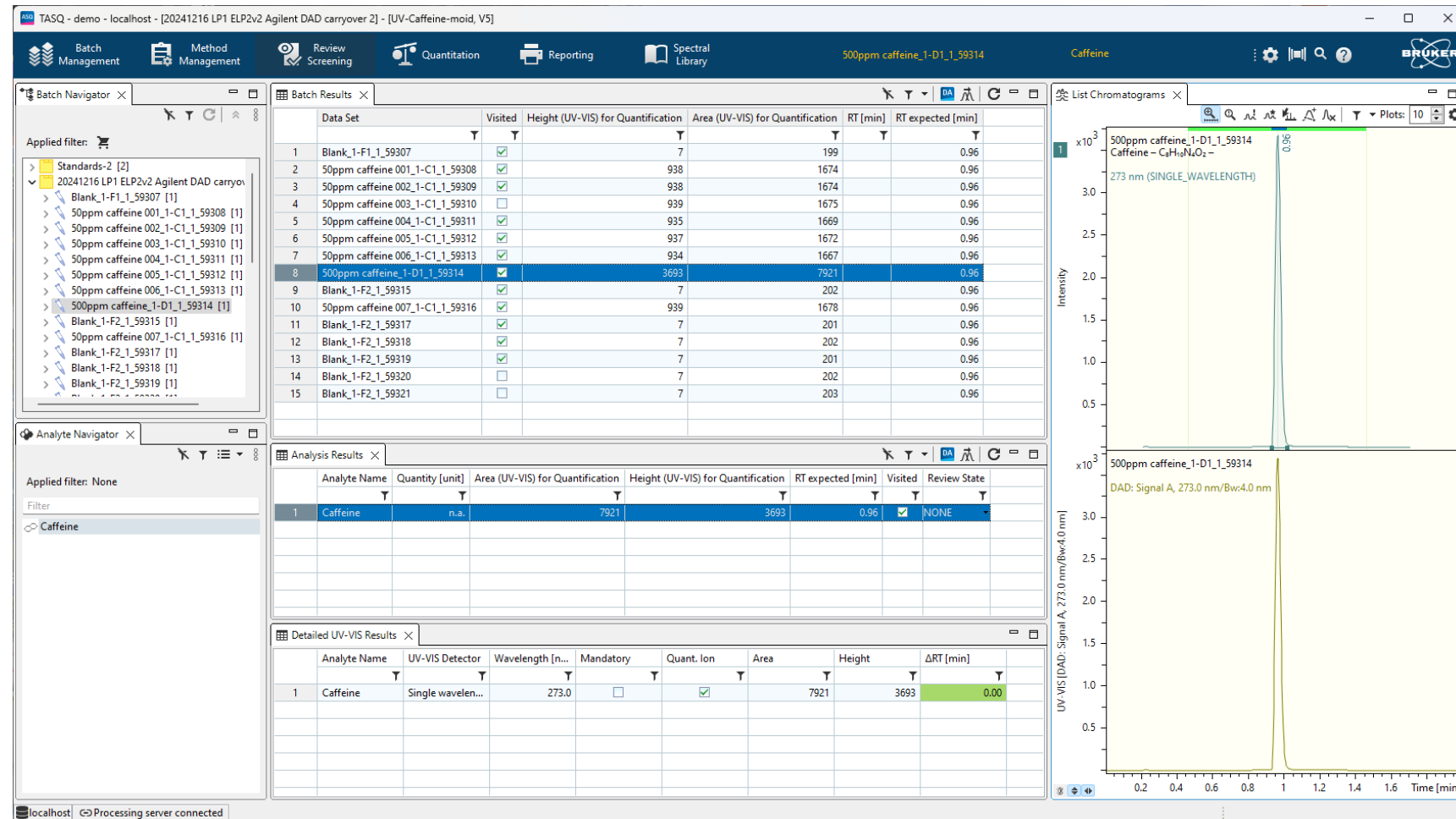
# TASQ 2026: Support GC w/o MS Data – GC Standard Mix

- Support:
  - GC FID traces
  - Manual integration
  - Quantification
    - GC Area
    - GC Height
  - Result columns



# TASQ 2026: Support UV-VIS Data w/o MS Data – Caffeine

- Support:
  - UV-VIS single wavelength
  - DAD – extracted UV-VIS chromatograms
  - Manual integration
  - Quantification
  - Result columns



The screenshot displays the TASQ software interface for a Caffeine analysis. The main window shows a list of data sets in the Batch Results table, with the selected entry '500ppm caffeine\_1-D1\_1\_59314' highlighted. The Analysis Results table shows the quantification of Caffeine, and the Detailed UV-VIS Results table provides specific parameters for the UV-VIS detector.

Data Set	Visited	Height (UV-VIS) for Quantification	Area (UV-VIS) for Quantification	RT [min]	RT expected [min]
1 Blank_1-F1_1_59307	<input type="checkbox"/>	7		199	0.96
2 50ppm caffeine 001_1-C1_1_59308	<input checked="" type="checkbox"/>	938	1674	1674	0.96
3 50ppm caffeine 002_1-C1_1_59309	<input checked="" type="checkbox"/>	938	1674	1674	0.96
4 50ppm caffeine 003_1-C1_1_59310	<input checked="" type="checkbox"/>	939	1675	1675	0.96
5 50ppm caffeine 004_1-C1_1_59311	<input checked="" type="checkbox"/>	935	1669	1669	0.96
6 50ppm caffeine 005_1-C1_1_59312	<input checked="" type="checkbox"/>	937	1672	1672	0.96
7 50ppm caffeine 006_1-C1_1_59313	<input checked="" type="checkbox"/>	934	1667	1667	0.96
8 500ppm caffeine_1-D1_1_59314	<input checked="" type="checkbox"/>	3693	7921	0.96	0.96
9 Blank_1-F2_1_59315	<input checked="" type="checkbox"/>	7		202	0.96
10 50ppm caffeine 007_1-C1_1_59316	<input checked="" type="checkbox"/>	939	1678	1678	0.96
11 Blank_1-F2_1_59317	<input checked="" type="checkbox"/>	7		201	0.96
12 Blank_1-F2_1_59318	<input checked="" type="checkbox"/>	7		202	0.96
13 Blank_1-F2_1_59319	<input checked="" type="checkbox"/>	7		201	0.96
14 Blank_1-F2_1_59320	<input type="checkbox"/>	7		202	0.96
15 Blank_1-F2_1_59321	<input type="checkbox"/>	7		203	0.96

Analyte Name	Quantity [unit]	Area (UV-VIS) for Quantification	Height (UV-VIS) for Quantification	RT expected [min]	Visited	Review State
1 Caffeine	n.a.	7921	3693	0.96	<input checked="" type="checkbox"/>	NONE

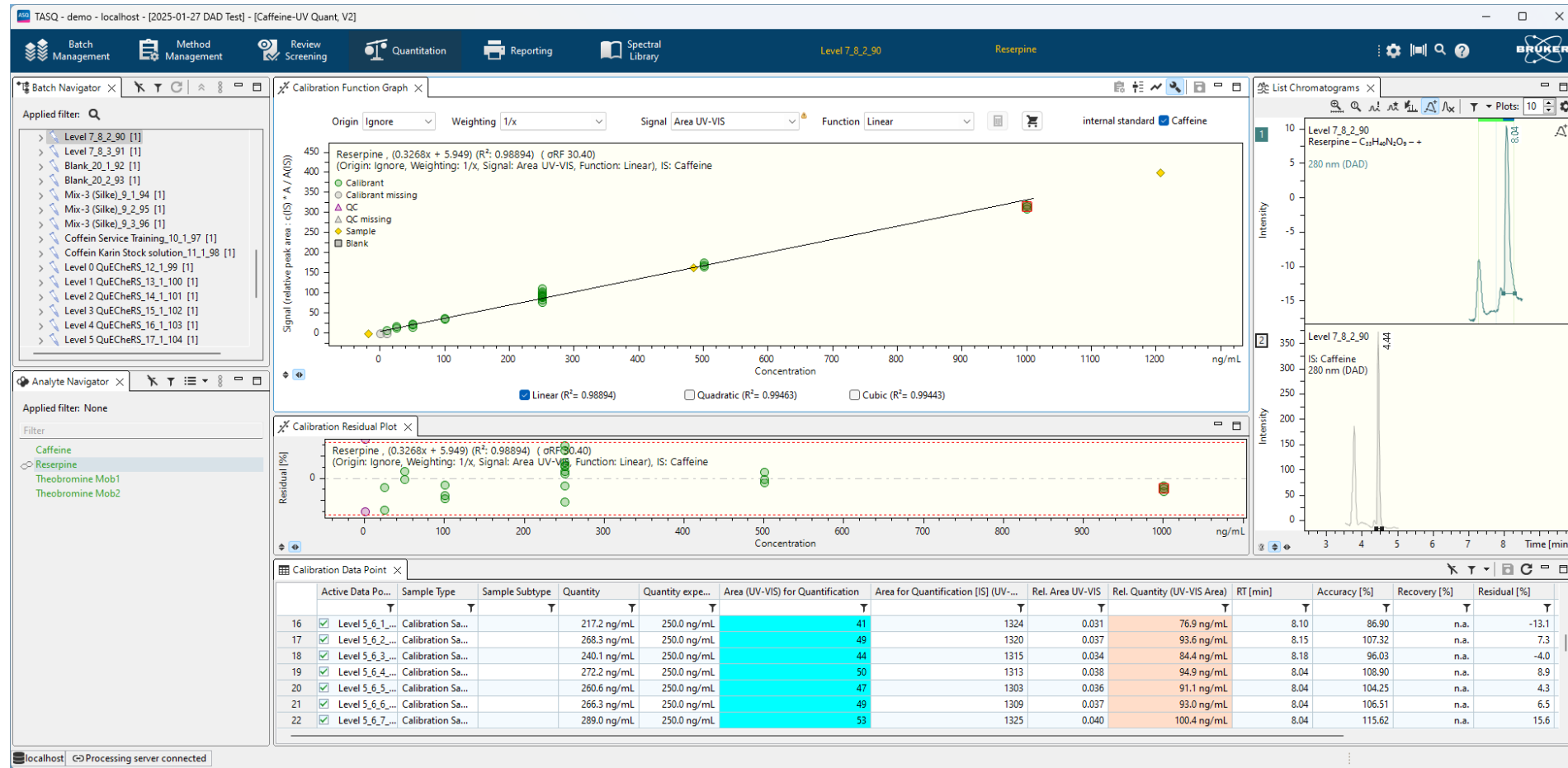
  

Analyte Name	UV-VIS Detector	Wavelength [nm]	Mandatory	Quant. Ion	Area	Height	ΔRT [min]
1 Caffeine	Single wavelen...	273.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>	7921	3693	0.00

The chromatograms on the right show the UV-VIS signal for Caffeine at 273.0 nm. The top plot is a single wavelength chromatogram, and the bottom plot is a DAD signal at 273.0 nm with a bandwidth of 4.0 nm. Both plots show a sharp peak at approximately 0.96 minutes.

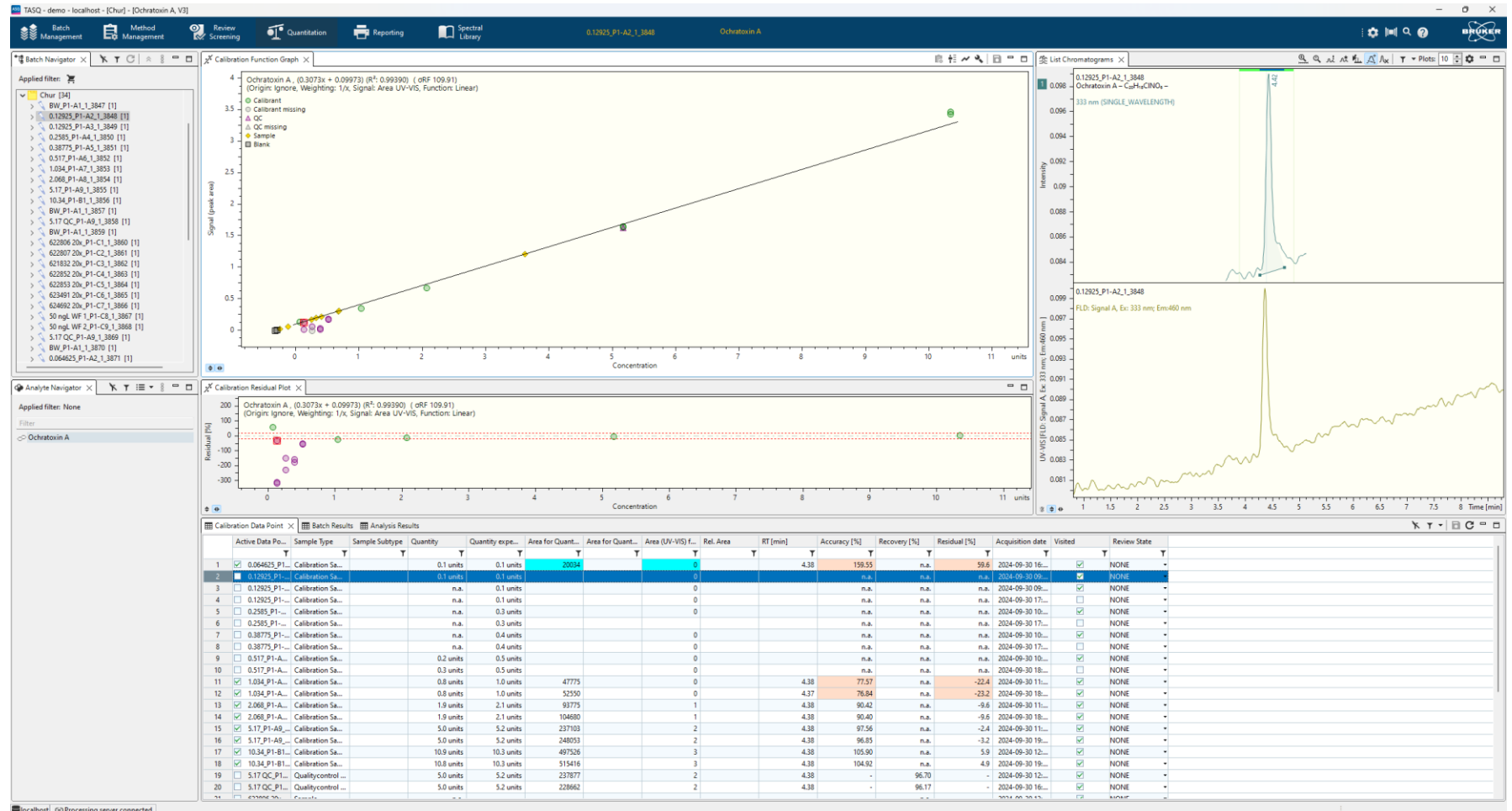
# TASQ 2026: Quantitation with UV-VIS Data with Internal Standard

- Dilution series of reserpine with IS: caffeine
- Manual integration of UV data supported



# TASQ 2026: FLD Data can be Handled as UV-VIS Data

- Interpret fluorescence detector data as UV-VIS detector
- Specify trace by using one of the two FLD wavelengths



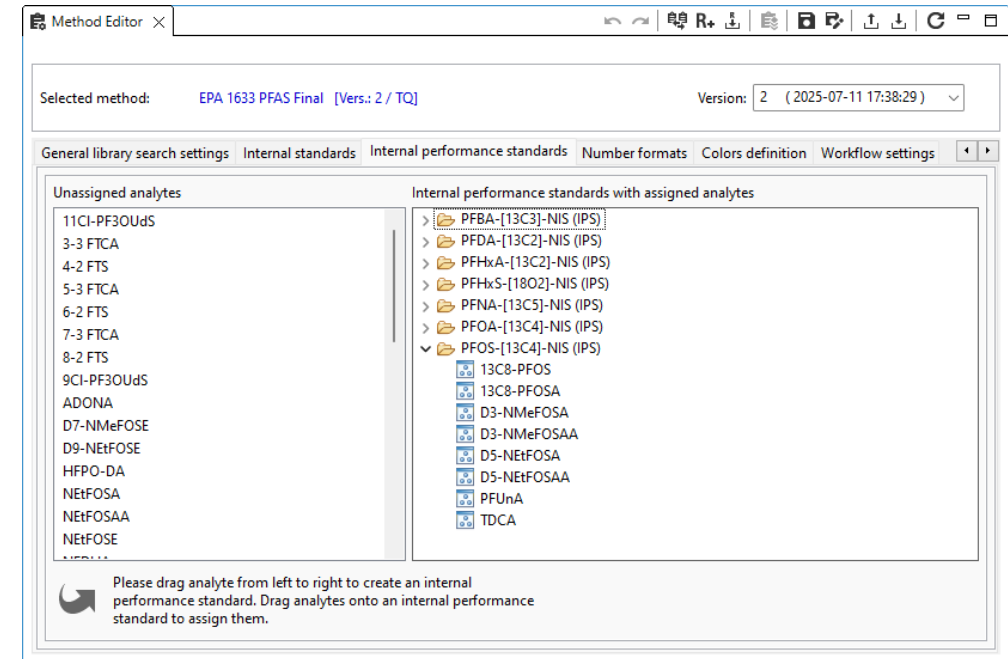
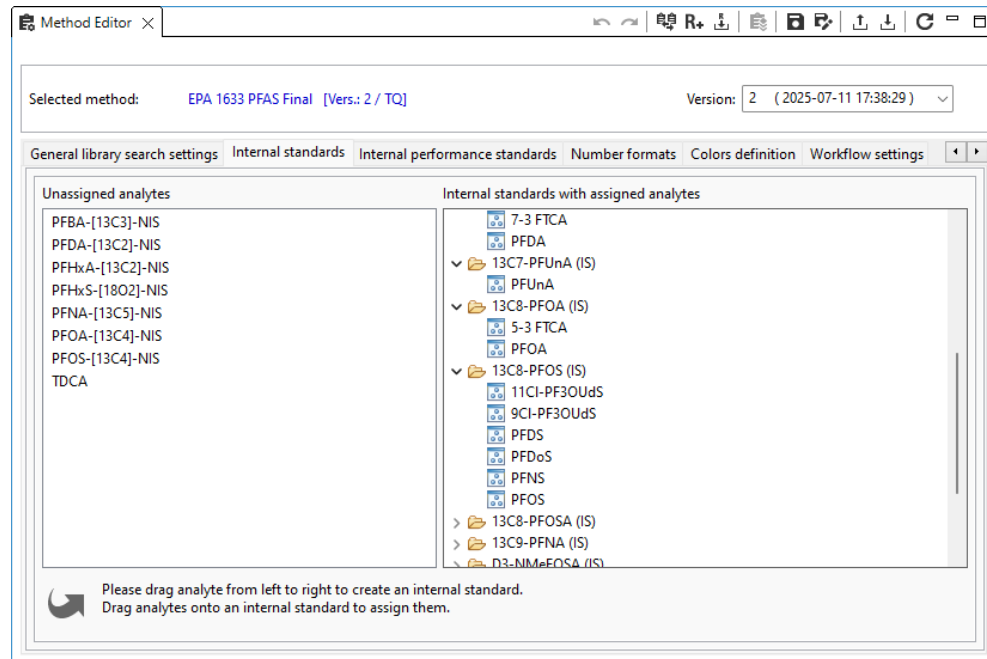
## TASQ 2026: Instrument Type Other

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- If data does not contain MS data but only UV-VIS or GC data assign instrument type Other to batch
- Adapt result views to show relevant columns in default configuration, hide MS specific columns
- Extended method profile settings with default settings for instrument type Other
- Changes to Detailed UV-VIS Result views: generalize to be used for GC data as well -> renamed to Detailed Other Result views. Show appropriate name depending on data. Detailed UV-VIS Results or Detailed GC Results view.
- Extend List Chromatograms view to show GC traces

# TASQ 2026: Extracted Internal Standard and Non Extracted Internal Standard

- Support for a second internal standard for EPA 533 and EPA 1633 – for PFOS an internal standard is spiked prior to sample preparation and one to the final test sample
- Known internal standard is used for specification of extracted internal standard
- Non extracted internal standard is declared as „Internal Performance Standard“



# TASQ 2026: Result Columns for internal performance standards

## Related Data

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Area for Quantification [IPS] (UV-VIS)

Area for Quantification[IPS]

IPS

Height for Quantification [IPS]

Height for Quantification [IPS] (UV-VIS)

Quantity expected [IPS]

RT(IPS) [min]

RT(IPS) [min] expected

Rel RT expected IPS

Rel. Area IPS

Rel. Height IPS

Rel. Quantity Area [IPS]

Rel. Quantity Height [IPS]

Rel.RT to IPS

Response IPS (Area IPS / c(IPS))

Response factor IPS/IS (Area / c)

$\Delta$ Rel.RT to IPS[%]

Area of UV-VIS chromatogram peak for internal performance standard

Area of internal performance standard

Name of of internal performance standard

Height of internal performance standard

Height for Quantification [IPS] (UV-VIS)

Quantity expected internal performance standard

Retention time of internal performance standard

Expected retention time of internal performance standard

Expected relative retention time

Area relative to internal performance standard

Height relative to internal performance standard

Relative Quantity Area [IPS]

Relative Quantity Height [IPS]

Retention time relative to internal performance standard

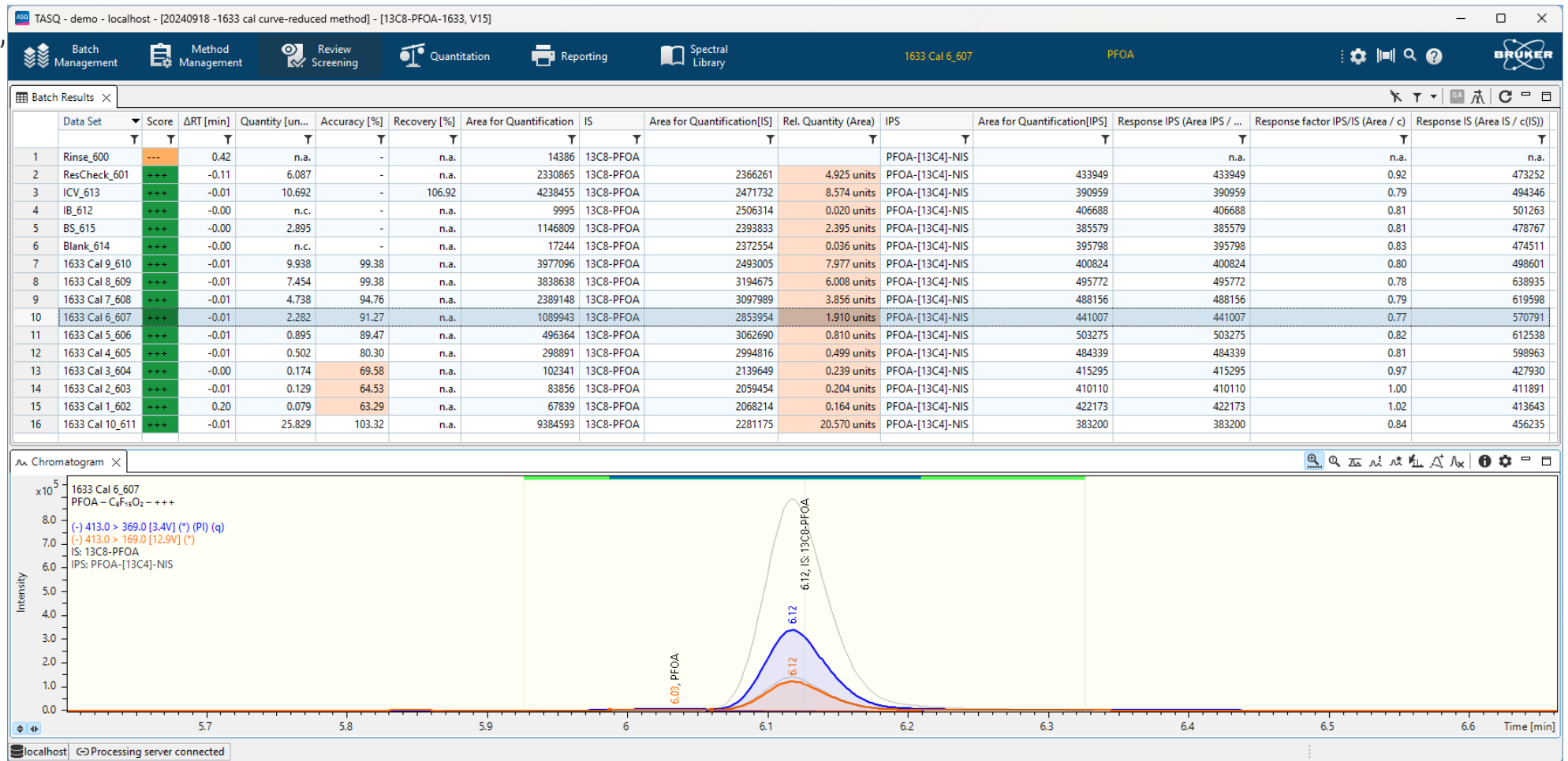
Response of internal performance standard (Area IPS / expected concentration IPS)

Response factor IPS / IS Area

Deviation of observed relative retention time to expected relative retention time in [%] to internal performance standard

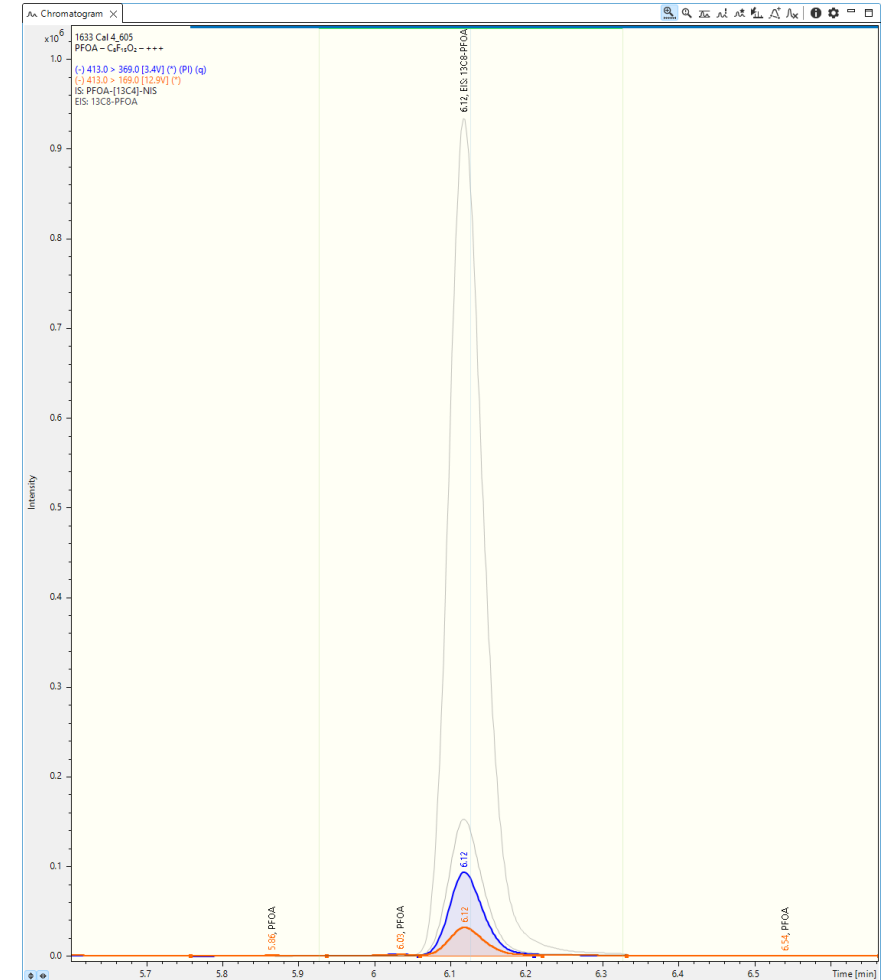
# TASQ 2026: Support EIS and IPS for PFOA in EPA 1633

- Columns for IS, IPS
- Name
- Areas
- Response
- Ratio IS/IPS



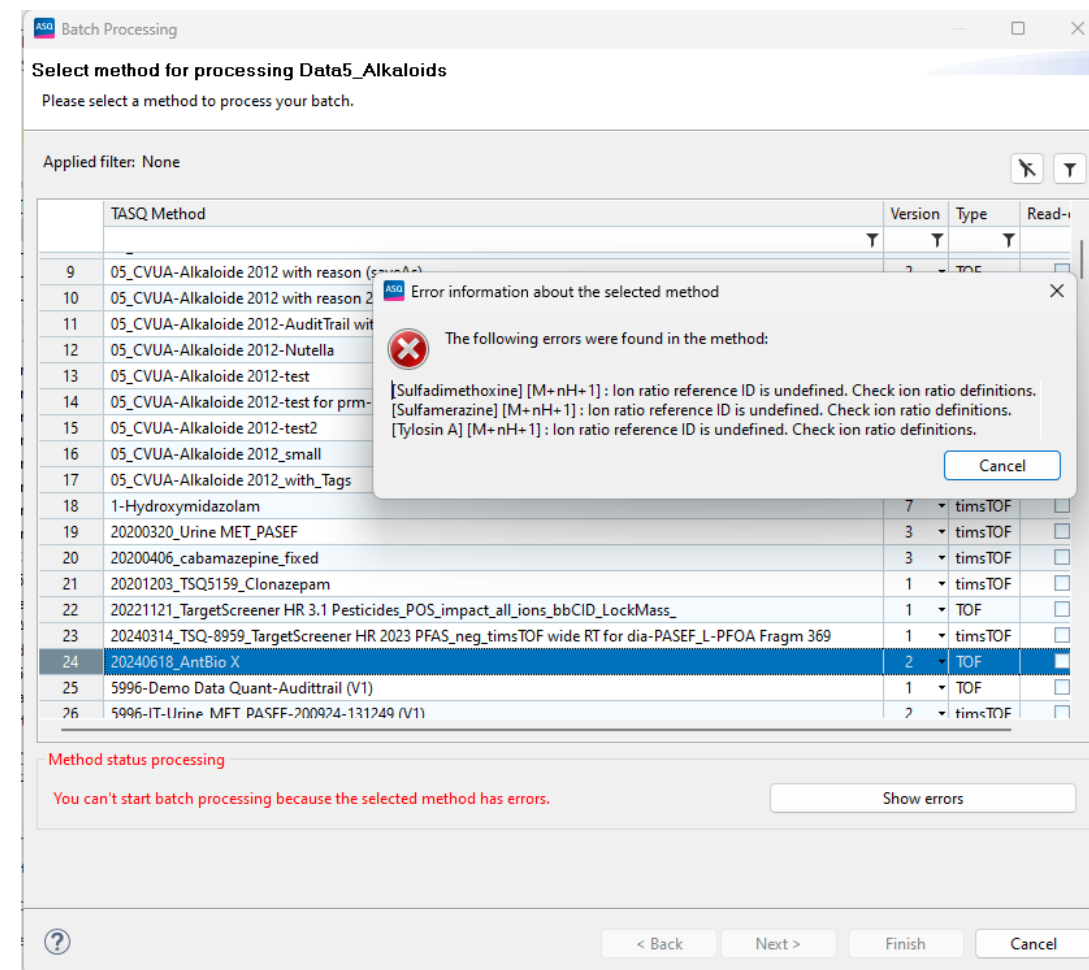
# TASQ 2026: Support for Additional Internal Standard

- Internal standard and internal performance standard traces are shown in chromatogram(s), mobilogram(s), and list chromatograms view



# TASQ 2026: Check Methods For Errors Prior To Processing

- Do not start processing of data if the processing method is not valid and contains errors
- Do list found errors to point out what needs to be corrected by user



The screenshot shows the 'Batch Processing' window in ASQ software. The main window is titled 'Select method for processing Data5\_Alkaloids' and contains a table of methods. An error dialog box is overlaid on the table, displaying the following error information:

**Error information about the selected method**

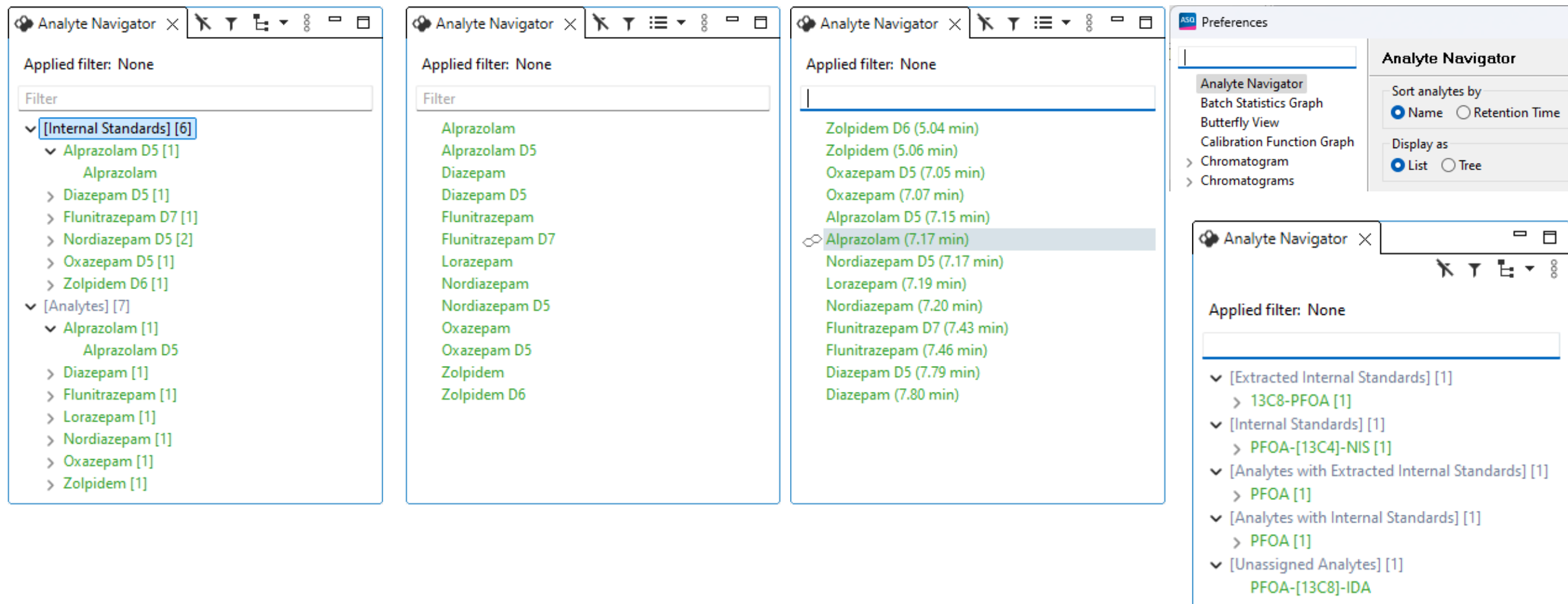
The following errors were found in the method:

- [Sulfadimethoxine] [M+nH+1]: Ion ratio reference ID is undefined. Check ion ratio definitions.
- [Sulfamerazine] [M+nH+1]: Ion ratio reference ID is undefined. Check ion ratio definitions.
- [Tylosin A] [M+nH+1]: Ion ratio reference ID is undefined. Check ion ratio definitions.

The dialog box has a 'Cancel' button. Below the table, the 'Method status processing' section shows a red message: 'You can't start batch processing because the selected method has errors.' and a 'Show errors' button. At the bottom of the window, there are navigation buttons: '< Back', 'Next >', 'Finish', and 'Cancel'.

TASQ Method	Version	Type	Read-i
9 05_CVUA-Alkaloide 2012 with reason 2	2	TOF	
10 05_CVUA-Alkaloide 2012 with reason 2	2	TOF	
11 05_CVUA-Alkaloide 2012-AuditTrail wit	2	TOF	
12 05_CVUA-Alkaloide 2012-Nutella	2	TOF	
13 05_CVUA-Alkaloide 2012-test	2	TOF	
14 05_CVUA-Alkaloide 2012-test for prm-	2	TOF	
15 05_CVUA-Alkaloide 2012-test2	2	TOF	
16 05_CVUA-Alkaloide 2012_small	2	TOF	
17 05_CVUA-Alkaloide 2012_with_Tags	2	TOF	
18 1-Hydroxymidazolam	7	timsTOF	
19 20200320_Urine MET_PASEF	3	timsTOF	
20 20200406_cabamazepine_fixed	3	timsTOF	
21 20201203_TSQ5159_Clonazepam	1	timsTOF	
22 20221121_TargetScreener HR 3.1 Pesticides_POS_impact_all_ions_bbCID_LockMass_	1	TOF	
23 20240314_TSQ-8959_TargetScreener HR 2023 PFAS_neg_timsTOF wide RT for dia-PASEF_L-PFOA Fragm 369	1	timsTOF	
24 20240618_AntBio X	2	TOF	
25 5996-Demo Data Quant-Audittrail (V1)	1	TOF	
26 5996-IT-Urine MFT PASEF-200924-131249 (V1)	2	timsTOF	

# TASQ 2026: Analyte Navigator – supports now IPS also



The image displays the Analyte Navigator interface in three different states, illustrating its flexibility in displaying data. Each window shows a list of analytes with their retention times and counts.

**Window 1 (Left):** Shows a tree view of internal standards and analytes. The [Internal Standards] section is expanded, showing Alprazolam D5 [1] (Alprazolam), Diazepam D5 [1], Flunitrazepam D7 [1], Nordiazepam D5 [2], Oxazepam D5 [1], and Zolpidem D6 [1]. The [Analytes] section is also expanded, showing Alprazolam [1] (Alprazolam D5), Diazepam [1], Flunitrazepam [1], Lorazepam [1], Nordiazepam [1], Oxazepam [1], and Zolpidem [1].

**Window 2 (Middle):** Shows a flat list of analytes: Alprazolam, Alprazolam D5, Diazepam, Diazepam D5, Flunitrazepam, Flunitrazepam D7, Lorazepam, Nordiazepam, Nordiazepam D5, Oxazepam, Oxazepam D5, Zolpidem, and Zolpidem D6.

**Window 3 (Right):** Shows a list of analytes with retention times: Zolpidem D6 (5.04 min), Zolpidem (5.06 min), Oxazepam D5 (7.05 min), Oxazepam (7.07 min), Alprazolam D5 (7.15 min), Alprazolam (7.17 min) (highlighted), Nordiazepam D5 (7.17 min), Lorazepam (7.19 min), Nordiazepam (7.20 min), Flunitrazepam D7 (7.43 min), Flunitrazepam (7.46 min), Diazepam D5 (7.79 min), and Diazepam (7.80 min).

**Preferences Dialog:** Shows the 'Analyte Navigator' section with options for 'Sort analytes by' (Name selected, Retention Time unselected) and 'Display as' (List selected, Tree unselected).

**Window 4 (Bottom Right):** Shows a different filter applied, displaying a list of extracted internal standards and analytes: [Extracted Internal Standards] [1] (13C8-PFOA [1]), [Internal Standards] [1] (PFOA-[13C4]-NIS [1]), [Analytes with Extracted Internal Standards] [1] (PFOA [1]), [Analytes with Internal Standards] [1] (PFOA [1]), and [Unassigned Analytes] [1] (PFOA-[13C8]-IDA).

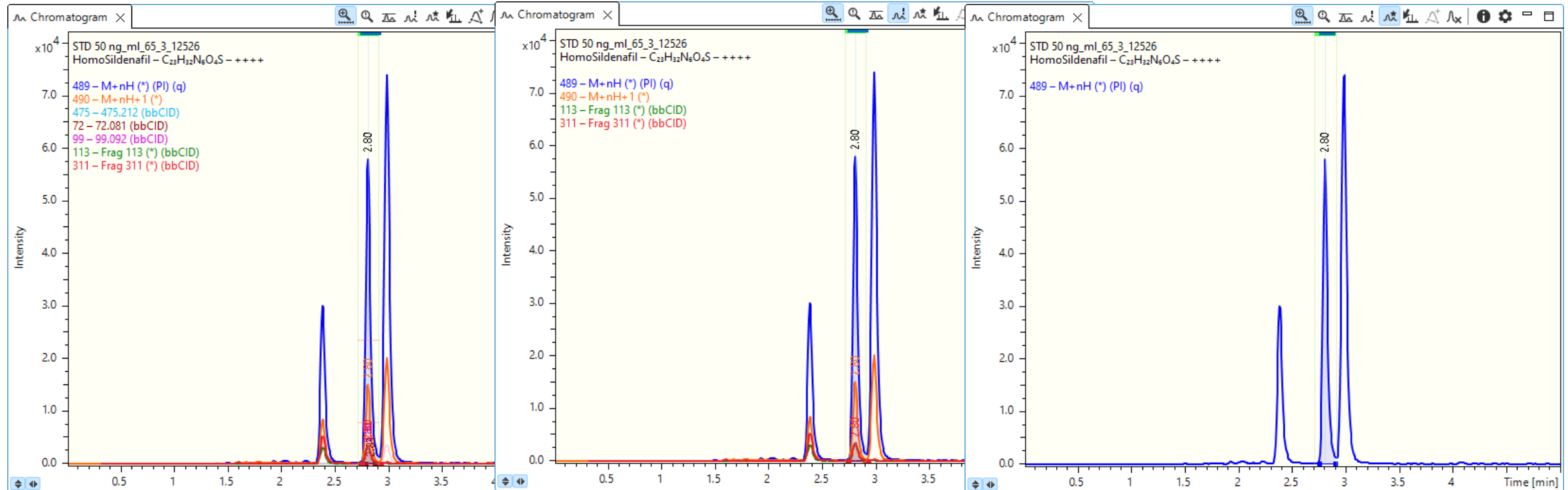
# TASQ 2026: New Columns in LIMS Export File

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Area UV Quantification  
Height UV Quantification  
Area Quantification  
Height Quantification  
Registry Number  
Dilution Factor  
Data Set Comment  
User Name  
Ion Ratio Valid Q  
Ion Ratio Valid Q1  
Ion Ratio Valid Q2  
Ion Ratio Valid Q3  
Ion Ratio Valid Q4  
Ion Ratio Valid Q5  
Area of internal performance standard  
Area of mobilogram peak for internal performance standard  
Height of mobilogram peak for internal performance standard  
Area of UV-VIS chromatogram peak for internal performance standard  
Height for Quantification [IPS] (UV-VIS)  
Quantity expected internal performance standard  
Expected retention time of internal performance standard  
Height of internal performance standard  
Retention time of internal performance standard  
Name of of internal performance standard  
Area relative to internal performance standard  
Height relative to internal performance standard  
Expected relative retention time  
Deviation of observed relative retention time to expected relative retention time in [%] to internal performance standard  
Retention time relative to internal performance standard  
Response of internal performance standard (Area IPS / expected concentration IPS)  
Response factor IPS / IS Area  
Sum of GC area values of all quantifier ions  
Sum of GC height values of all quantifier ions  
Area GC relative to internal standard  
Height GC relative to internal standard  
Relative quantity based on internal standard  $c = (\text{Signal Area for Quantification GC} / \text{Signal IS GC}) * c_{IS}$   
Relative quantity based on internal standard  $c = (\text{Signal Height for Quantification GC} / \text{Signal IS Height GC}) * c_{IS}$

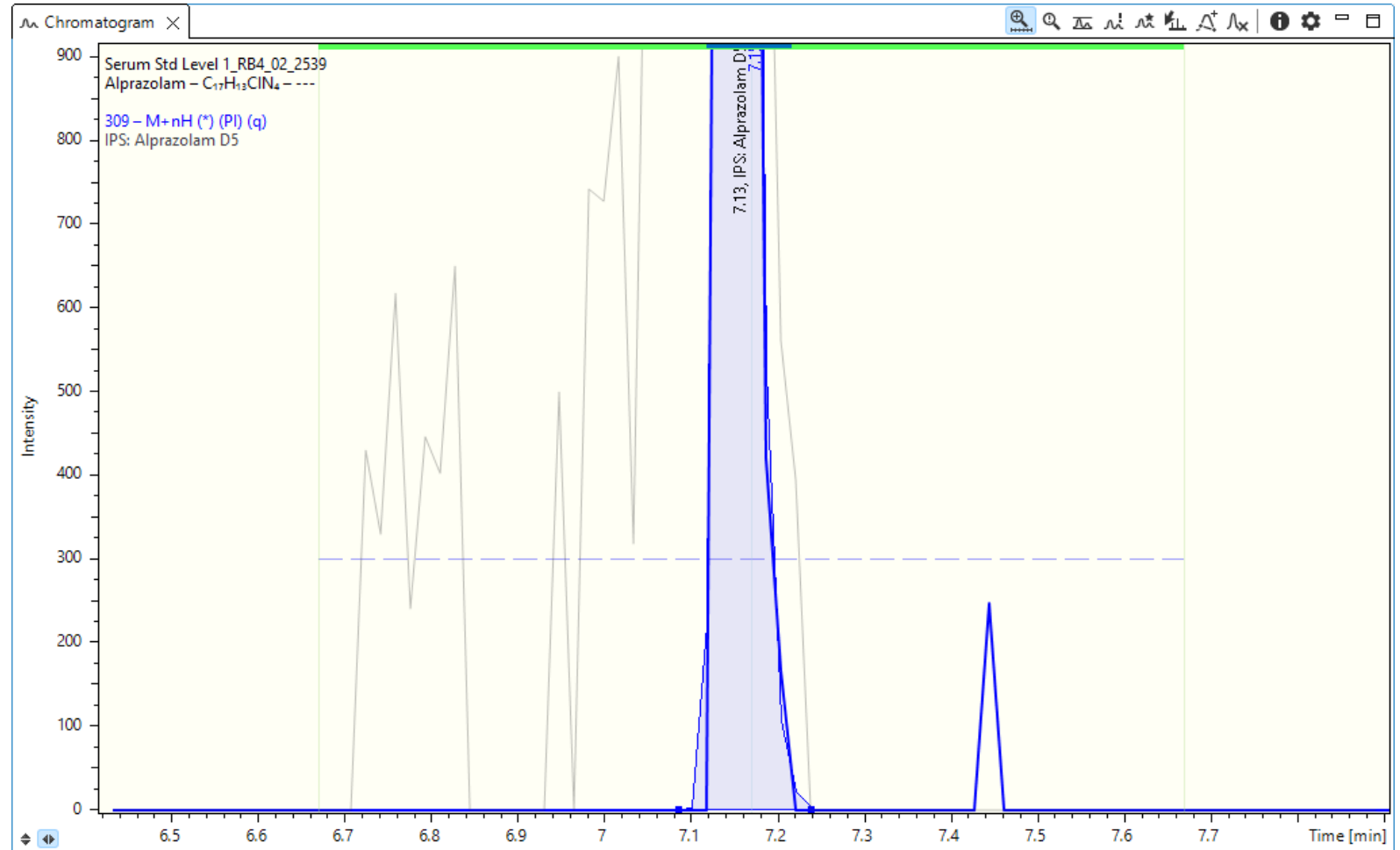
# TASQ 2026: Enhance Options for Chromatogram View

- Added toggle buttons to show:
- Chromatograms of mandatory ions or quantitation ions only



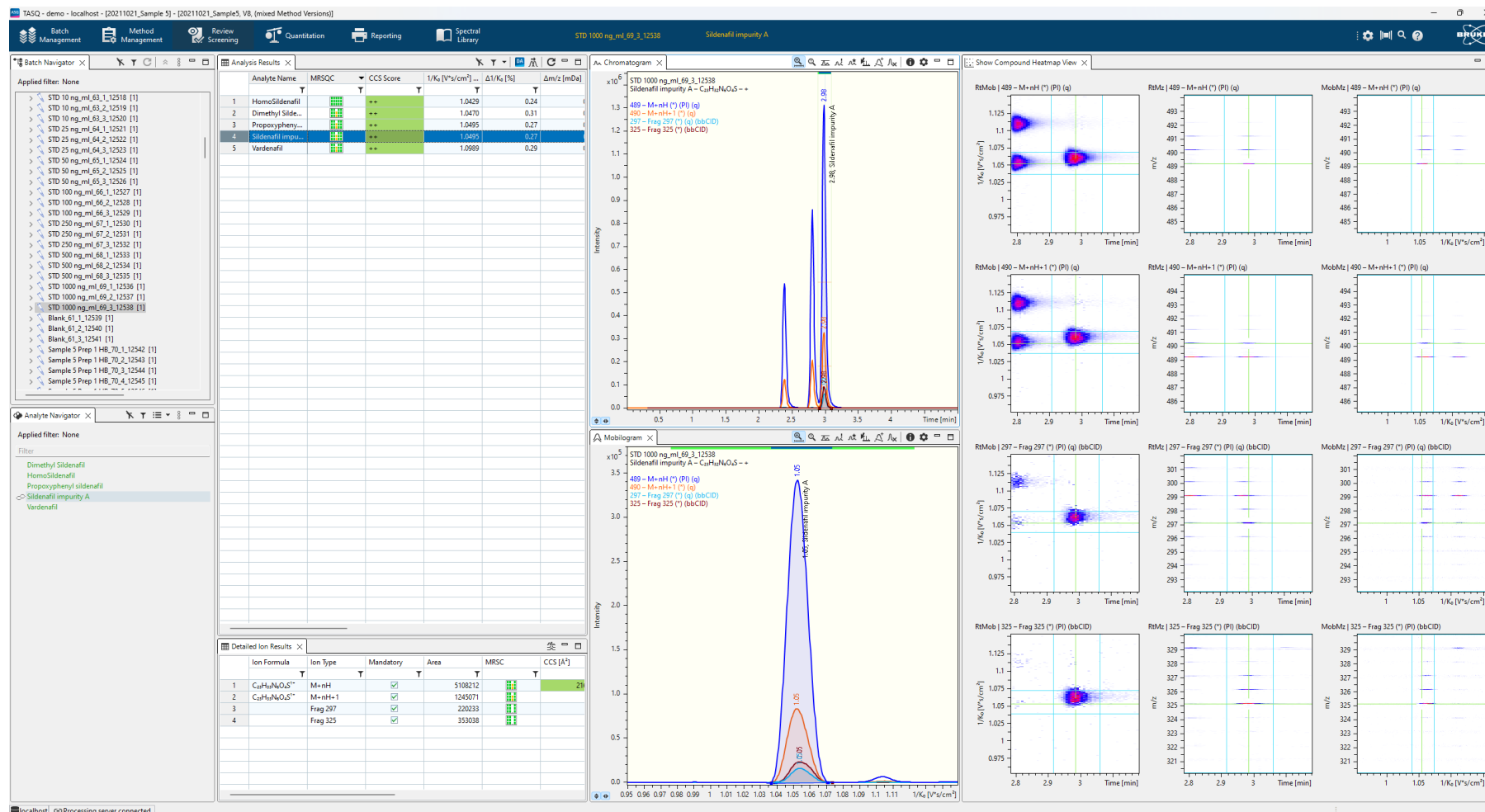
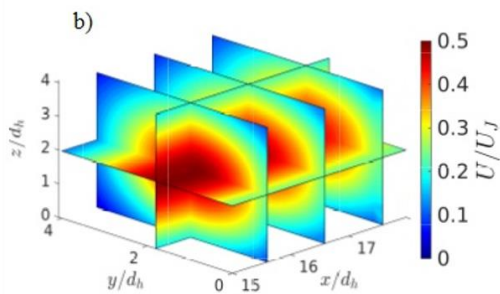
# TASQ 2026: Chromatogram View Overlay Intensity Threshold

- Optionally overlay a horizontal line for the intensity threshold as specified in the processing method



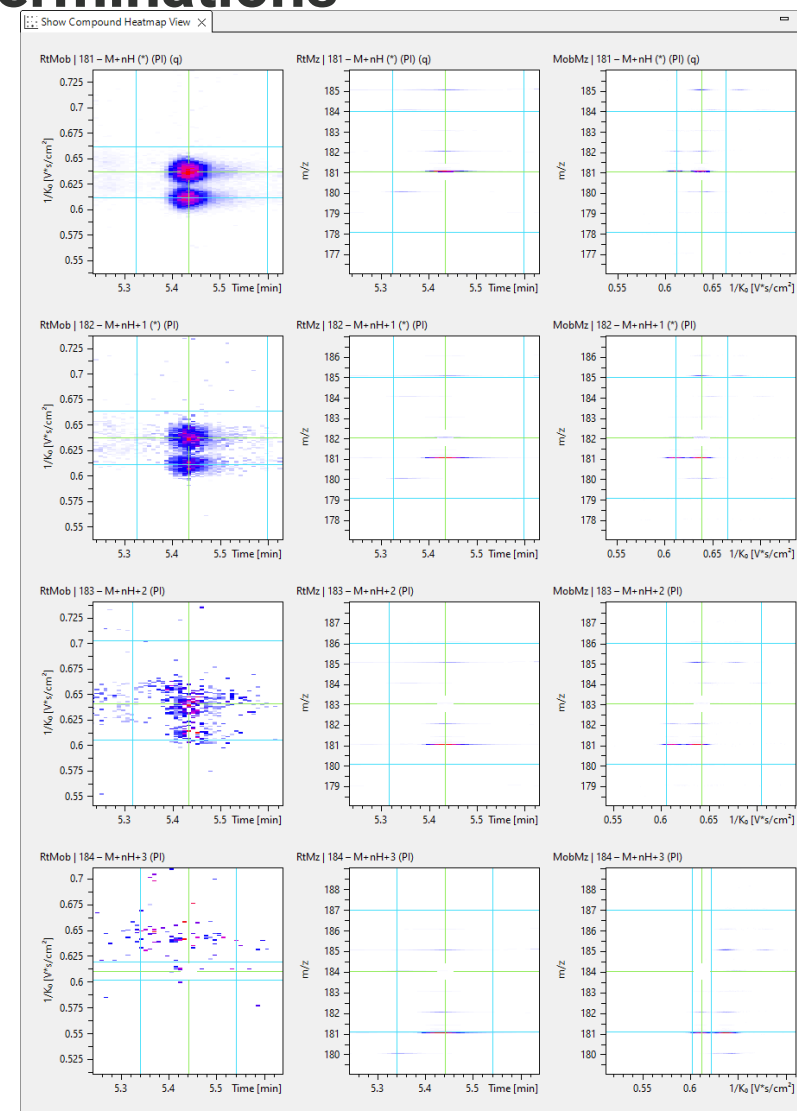
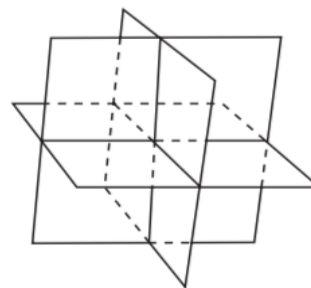
# TASQ 2026: Show Compound Heat Map View for Determinations

- Get more insights into data than with 1D chromatograms or mobilograms
- Will be calculated on selection change of determination
- Illustration:



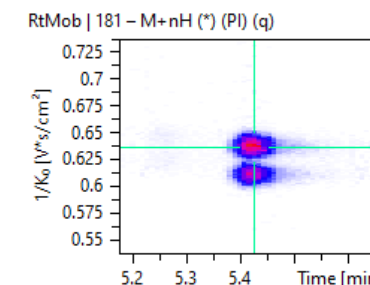
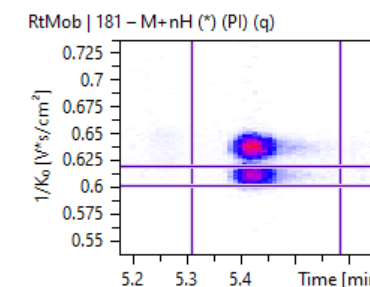
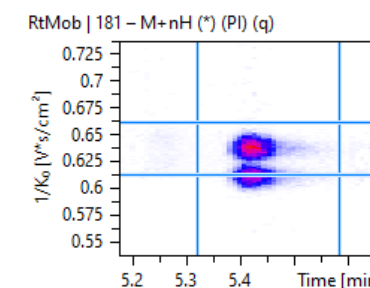
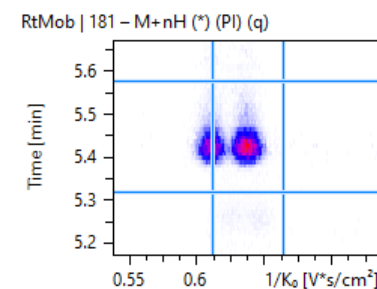
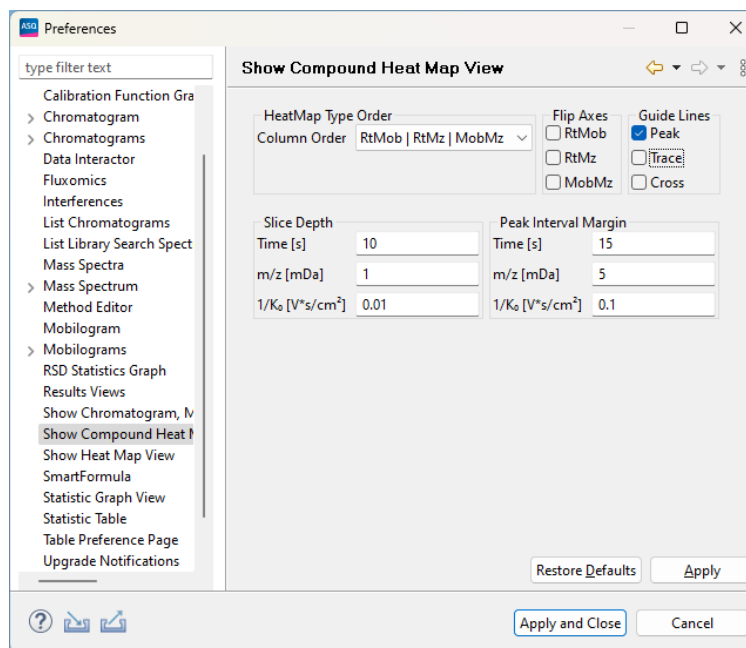
# TASQ 2026: Show Compound Heat Map View for Determinations

- Show heatmaps for each ion in all three main projections
- RT vs mobility
- RT vs m/z
- m/z vs mobility
- Drag and drop of columns possible
- Option to flip axis
- Overlay bounds used for trace generation
- Overlay bound to show peak ranges



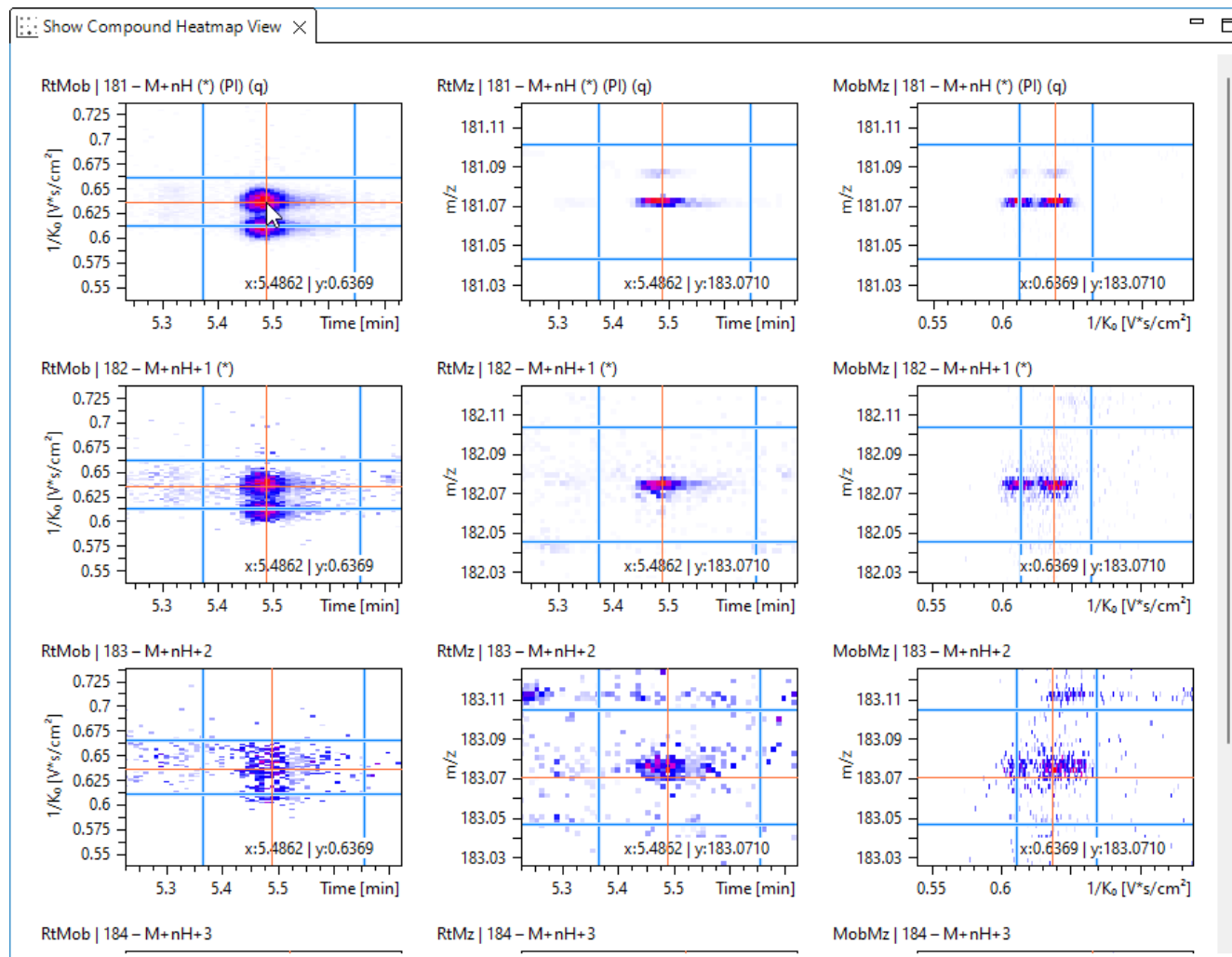
# TASQ 2026: Show Compound Heat Map View for Determinations

- Preferences to configure order and orientation of faces
- Specify which guidelines shall be shown – detected peak start/end, intervals for trace generation, peak apex position
- Specify which thickness a slice shall have in z direction
- Specify additional margin relative to peak start/end or tolerances specified in processing method



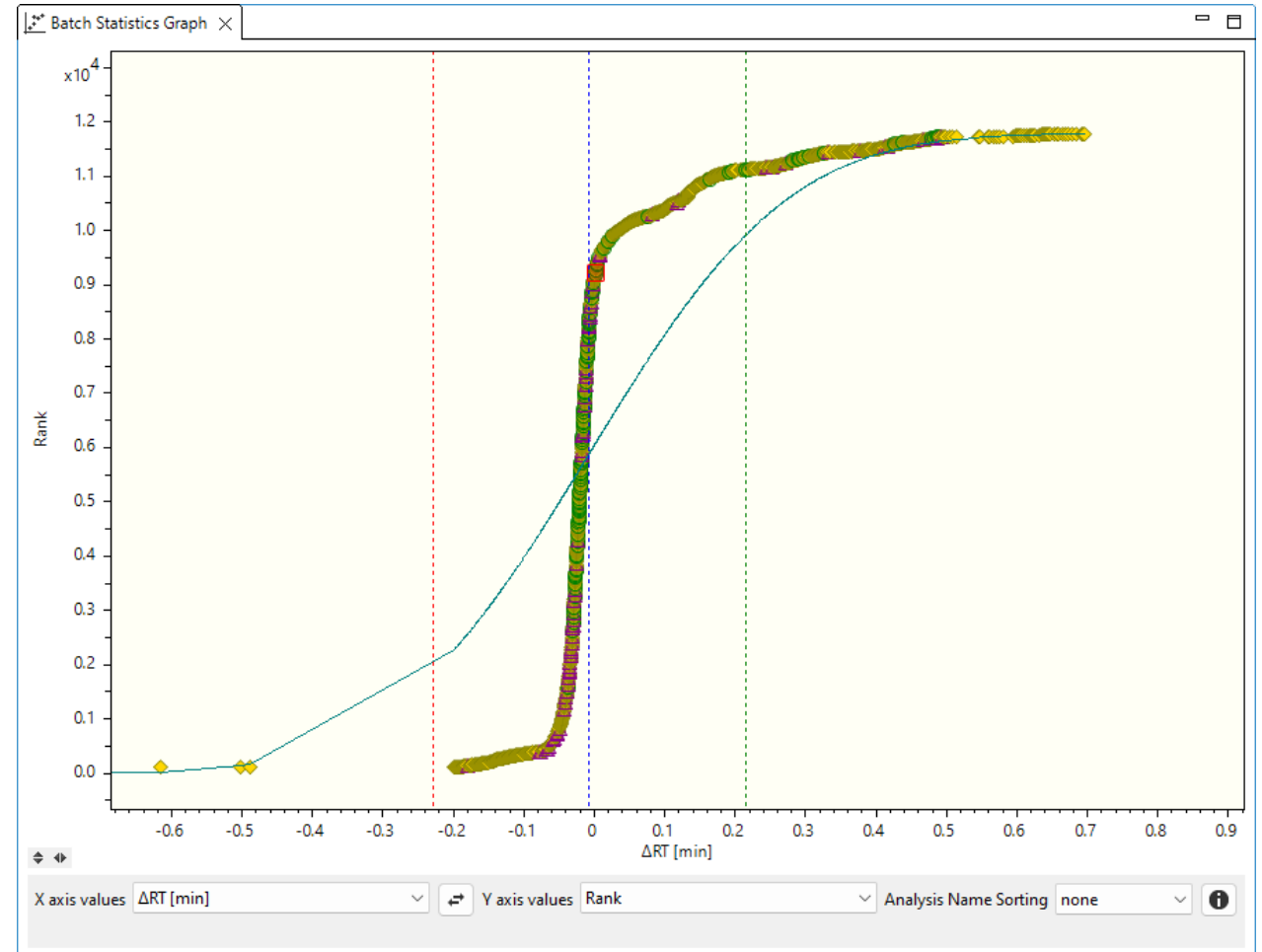
# TASQ 2026:

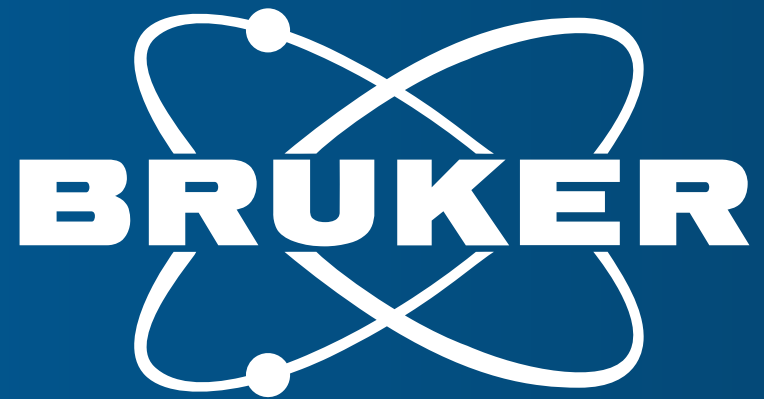
- Show guidelines through current mouse position simultaneously in all views



## TASQ 2026: Batch Statistics Graph - Rank

- Show the rank of a property
- Overlay a cumulative probability assuming a normal distribution with mean and standard deviation of the selected property
- Show guidelines for mean and mean  $\pm$  sd
- Easily swap x and y property to reflect the graph





Innovation with Integrity