TASQ 2026B

TASQ 2026b: What is new?

TASQ 2026B: Main Features

- REST API
  - Create batch for acquisitions and start acquisition
  - Monitor batch under acquisition
  - Retrieve determinations for acquired batch
- Allow user defined QC methods / batches in TASQ QSee Performance Test Tool
- Show MS/MS spectra for selected MS/MS event in Show MS view
  - Select a MS/MS event in Chromatogram view / Heat Map view
- Perform manual integration in Heat Map view / Compound Heat Map view
- Support disentanglement of TASQ and tqControl – Enable method creation and synchronisation

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TASQ 2026B: Minor Features

- Support Enhanced Linear Mobility Calibration for timsTOF
- CCS Predict for selected analytes
- Add analytes to a TASQ processing method by file import
- Retrieve batches by TASQ processing method
- Assign internal / performance standard in analyte settings table in method editor
- Improvements in internal / performance standard tab in method editor
- Improved and more relaxed error handling for inconsisten settings in TASQ method

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TASQ 2026B: Switched to Compass Platform 11

- Compass Platform 11
  - Brings updated components with less vulnerabilities
  - Improved user interface for definition of user roles and user action rights
  - Setup of Compass Server gives a warning if the data base location is on a HDD
  - Improved handling to keep existing data base if compass server was uninstalled first
  - Automatic update of postgre data base SW product
  - Improved installer for compass server selector -> should improve performance of setups which install the compass server selector
  - Provides a new tray configuration for Elute Splitflow autosampler
  - Bug fixes

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TASQ 2026B: REST API

- Login / Logout
- Batches
  - Create batch from file
  - Create batches
  - Search batches with criteria
  - Retrieve batch by ID
  - Retrieve batches by TASQ method ID
  - Start acquisition of batch with ID
  - Process Batch
- Methods
  - Export -> .tasqMethod
  - Export As TSV -> .tsv
  - Validate TASQ method <- .tasqMethod
  - Import TASQ method <- .tasqMethod
  - Import TASQ method <- .tsv, .tqml
  - Retrieve all method profiles
  - Retrieve method by ID, name, batch ID
  - Retrieve analytes from a TASQ method
  - Search TASQ methods

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TASQ 2026B: REST API

- Results
  - Determinations of data set
  - Determinations of analyte in batch
  - Determination by id
  - Retrieve chromatogram, mobilogram, MS spectrum
  - Retrieve calibration functions by analyte id
- Reporting
  - Retrieve reports for analysis
  - Retrieve reports for batch
  - Retrieve all batch report layouts
  - Retrieve all analysis report layouts
  - Create new report for batch with layout
  - Create new report for analysis with layout
  - Download a report
  - Retrieve creation status of a report

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TASQ Future Version: REST API

- In a future version the REST API will be extended to support:
  - Import brkrar file
  - Export brkrar file
  - Import acquired raw data as batch
  - Extend a batch

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TASQ 2026B: Prerequisites for Usage of REST API

- User has to obtain a WIBU license: 1925070
- User has to create an API token in administration preferences
- User has to configure a development environment
  - User may use Python with or without a Jupyter Notebook
  - User has to install TASQ REST API component
  - User has to get Compass Server Certificate
- There is a How To together with example Juypyter Notebook files demonstrating key features

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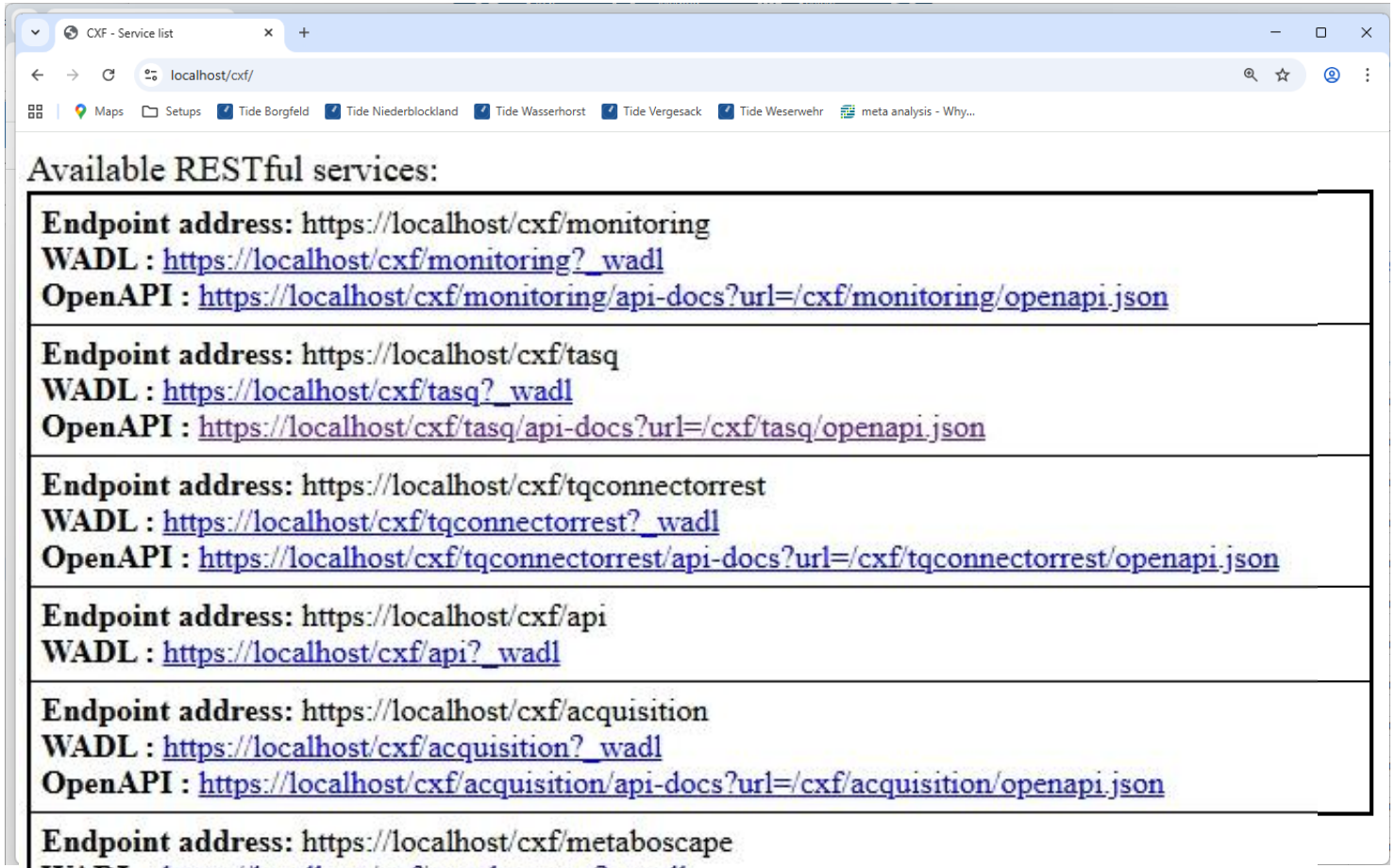
TASQ 2026B: SWAGGER UI https://localhost/cxf

- Swagger UI is mainly meant to be a source for documentation of the RESTA API available from Compass Platform and the installed applications
- A user who wants to implement against the published interfaces finds all relevant information and is able to test indvidual REST API methods
- It‘s not meant to be used for day to day work



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TASQ 2026B: Other REST APIs Available from Compass Server

- Monitoring: Used for monitoring Compass Server
  - get available stations on the Compass Server
  - get status and content of the HyStar acquisition queue of a specific station
  - get content of Compass Server Event Log (only available starting from Compass Server 12.0)
- Acquisition: Used for controlling HyStar acquisition, focuses on basic HyStar acquisition workflows and does not allow creating batches for TASQ / MetaboScape, BPC workflows
  - get list of previously used batch tags
  - get list of available sample types and associated sample subtypes
  - search for existing batches
  - create new batches and analyses
  - get detailed information on specific batch and analyses
  - edit existing batches and analyses
  - add or remove batches to and from HyStar acquisition queue
  - control acquisition queue (suspend, resume, stop)

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TASQ 2026B: Jupyter Notebook as Python Scripting Environment for Rapid Development and Enthusiastic Users

- It‘s easy – try it!
- Most simple setup would be to install PyCharm community edition which is free to use
  Disable all notifications for statistics sent to IntelliJ
  Disable the AI features offered by IntelliJ
- Just install it and use it, PyCharm will take care of installing latest Python and starting Jupyter server
- Create a new Jupyter notebook -- Create a localhost.cert file
- Copy code from example notebook or adapt example notebook to your local setup -> token, batch names, method names,…
- AI is also very helpful for creating code snippet – Use company provided AI tools and version.
- Handling of the data structures is a little bit complicated, you have to gather experience. But don‘t be afraid.

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TASQ 2026B: Demo Jupyter Notebooks for REST API

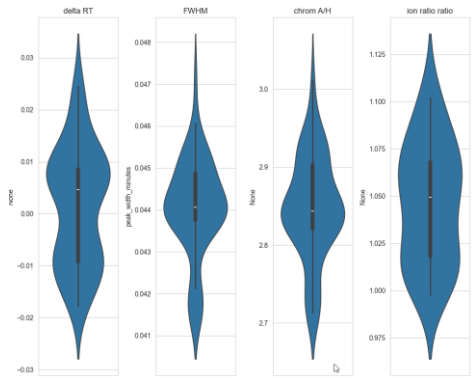
Code | Markdown

TASQ Process Batch

Authentication

Enter Compass user API Key for "api_key"
Enter REST API url for "url"
Enter path to Compass certificate for "certPath"

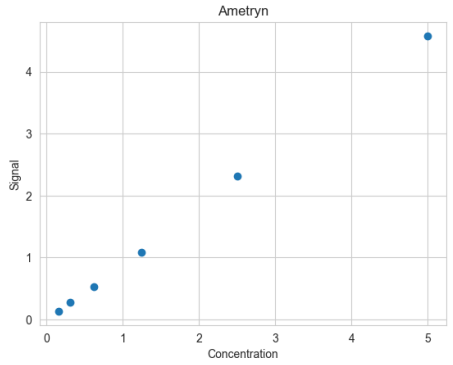
```
method_name = 'triazine-L-blubfasel'
search_batch_name = "Triazine"

```



Retrieve most important meta data for each data set

```
analyses_df = df[[ "name", "sample_type", "calibration_level", "dilution", "injection_volume", "id", "tasq_method_id"   ]]
analyses_df.head()
```

	name	sample_type	calibration_level	dilution	injection_volume	id	tasq_method_id
0	hesi_1-28-2013_9-57-19 pm_l1 triazine	CALIBRANT	0	1.0	30.0	04cf0e42-4b08-4e4a-a70c-16331593c640	None
1	hesi_1-28-2013_10-04-30 pm_l2 triazine	CALIBRANT	0	1.0	30.0	ebb71ca5-3ac9-41ed-98a9-a6951316d0e5	None
2	hesi_1-28-2013_10-11-42 pm_l3 triazine	CALIBRANT	0	1.0	30.0	1e71002b-a297-4e10-80ef-6837e1f1d8ae	None
3	hesi_1-28-2013_10-18-54 pm_l4 triazine	CALIBRANT	0	1.0	30.0	02036c7e-52a9-4ba5-9272-7912e49e8f52	None
4	hesi_1-28-2013_10-26-06 pm_l5 triazine	CALIBRANT	0	1.0	30.0	f99c8094-3deb-425b-867c-3ec929426b1c	None



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TASQ 2026B: Disentanglement tqControl ← → TASQ

- Create a processing method for method set of TQ batch based on acquisition method
- Update retention times of RT in acquisition method and update processing part in method set
- Update analytes and ions in processing method according to the acquisition method of method set in TQ batch

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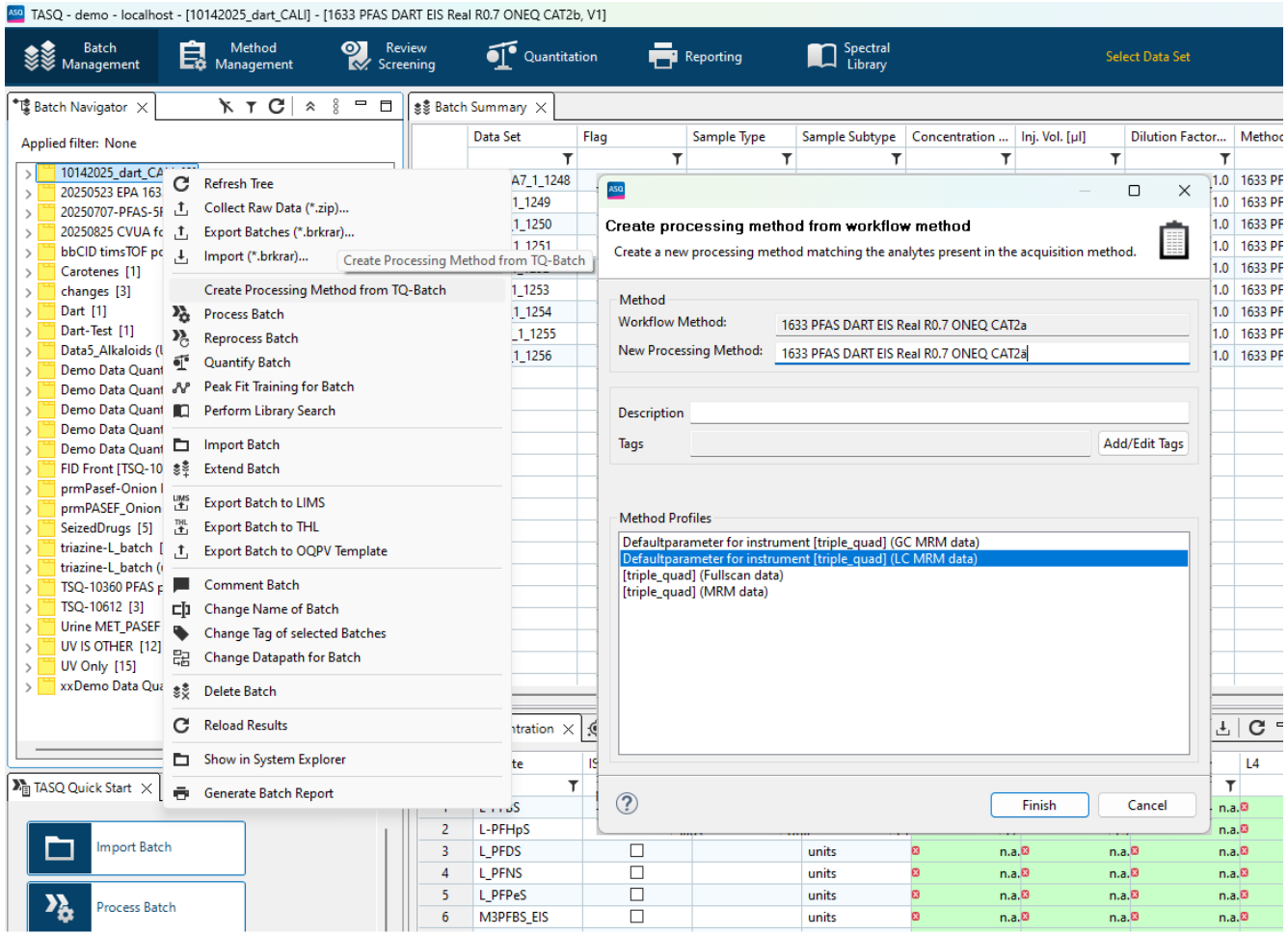
TASQ 2026B: Disentanglement tqControl ← → TASQ

- Create a processing method for workflow method of TQ batch
- User can specify
  - Name of processing method
  - Descripiton
  - Tag
- User has to choose method profile for default parameters



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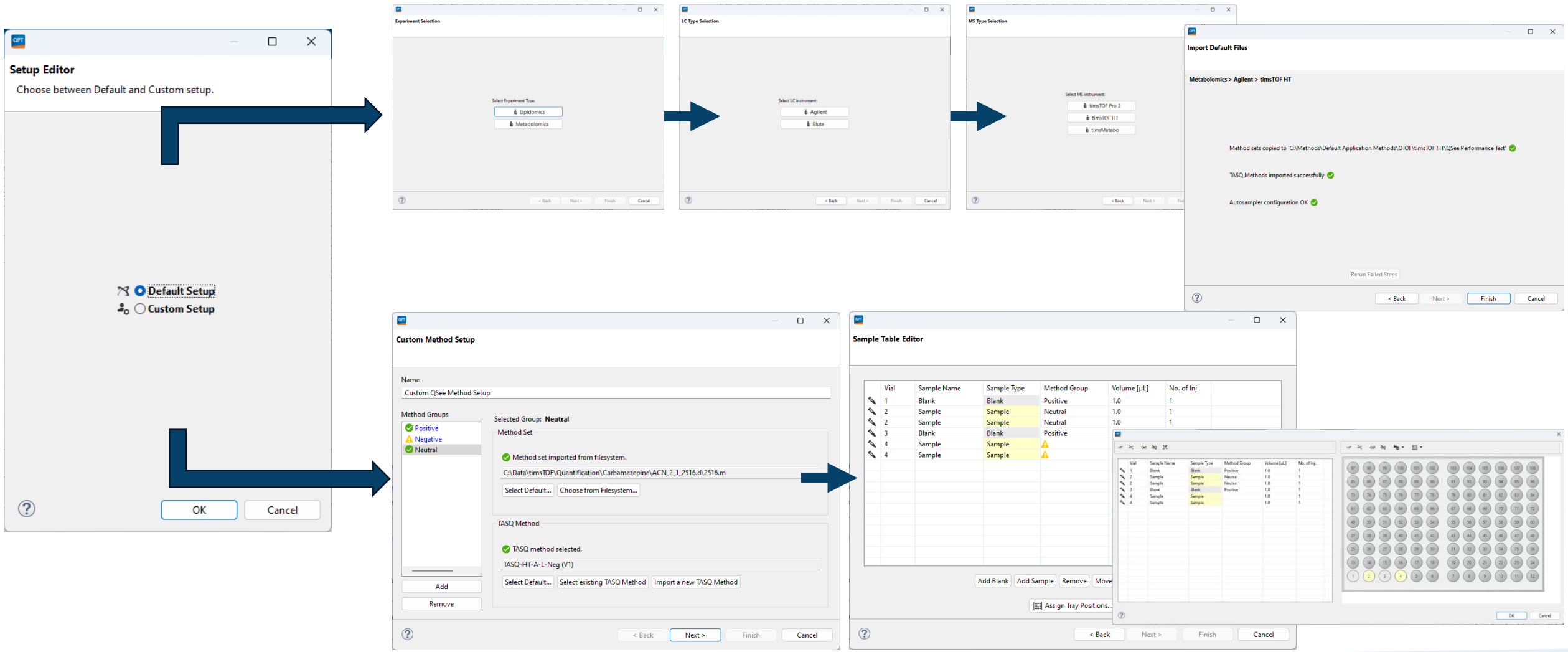
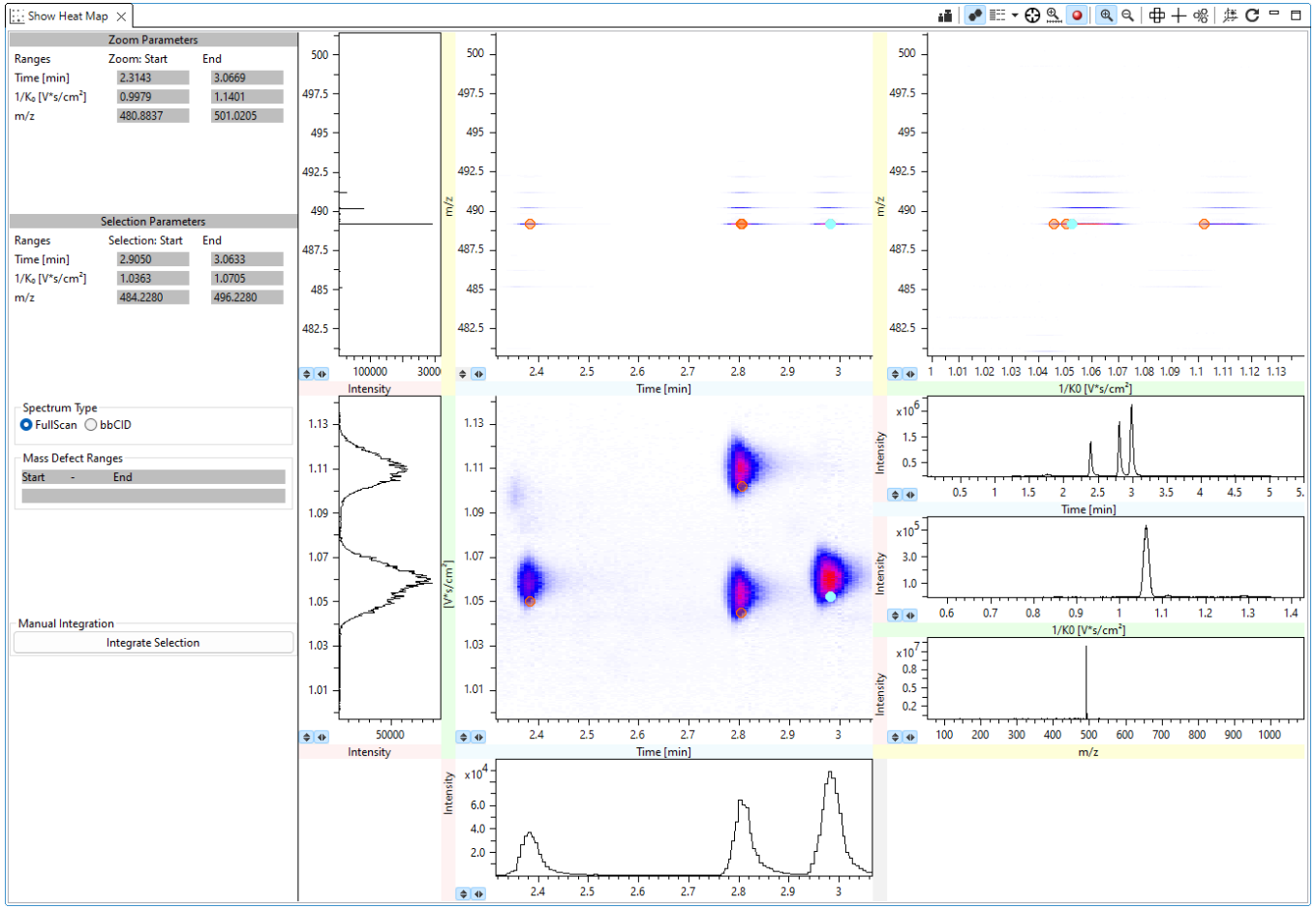
TASQ 2026B: QSee Performance Test Tool – Performance Test Setup – Factory Setup or User Defined Custom Setup



TASQ 2026B: Show Heat Map improved

- Reworked Show Heat Map view
- Scales are aligned neatly
- Vertical axis labels improved
- Performance loading heat maps and projections improved
- First implementation for manual integration available -> results send to Show MS, Show Chromatogram, Show Mobilogram views
- Moving picture by dragging the x-axis or by scrolling with mouse wheel
- Enlarge picture with mouse wheel



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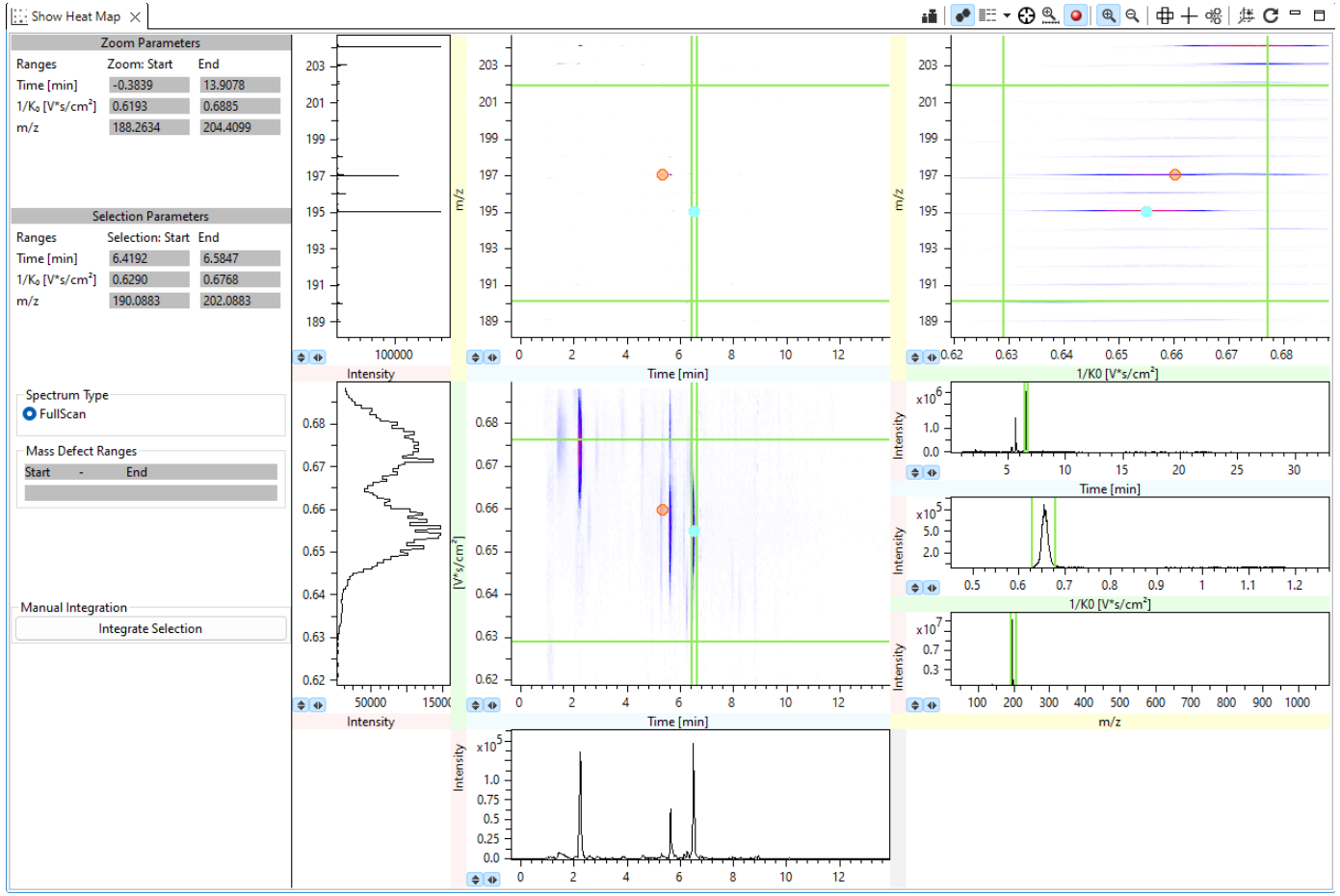
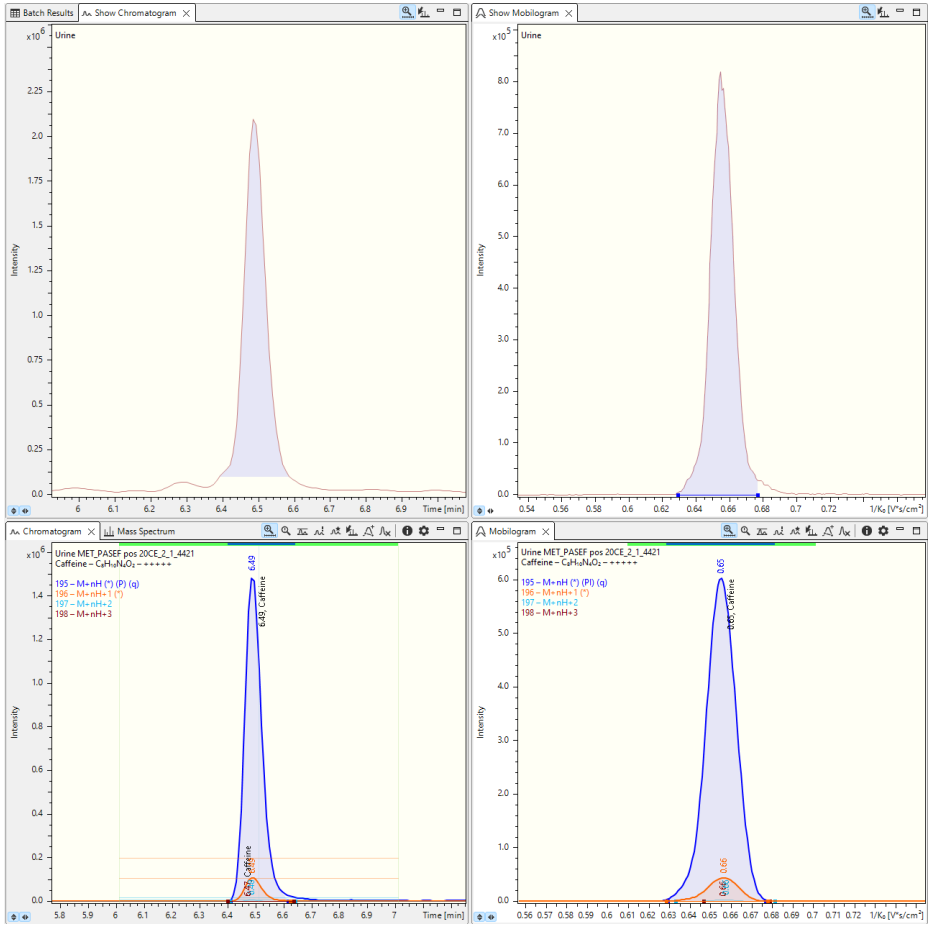
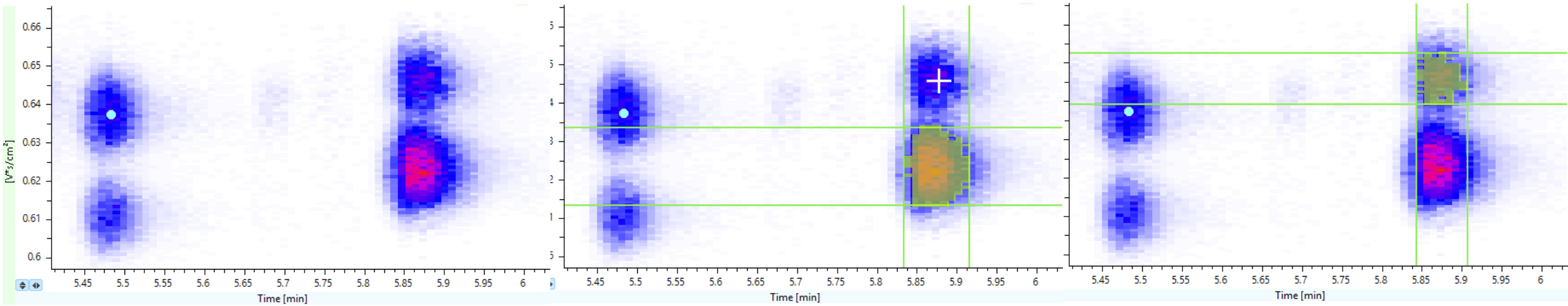
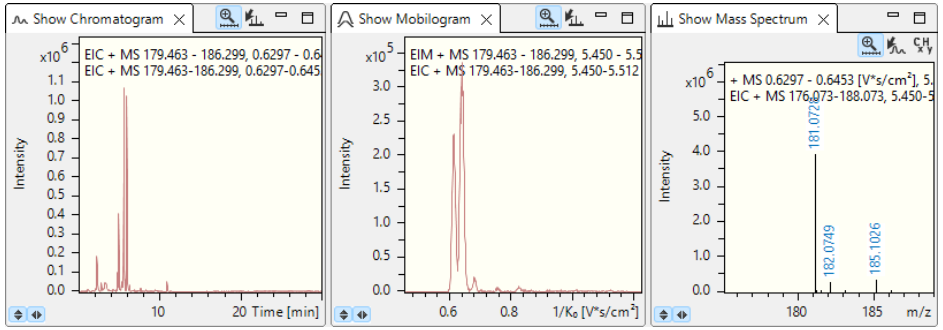
TASQ 2026B: Heat Map View: Manual Integration

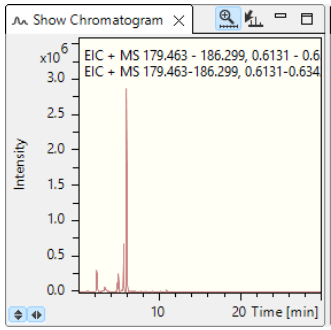


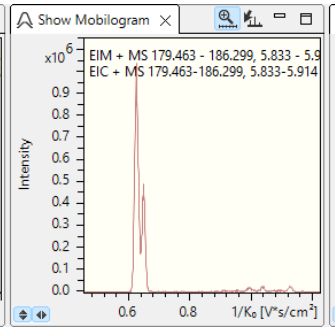


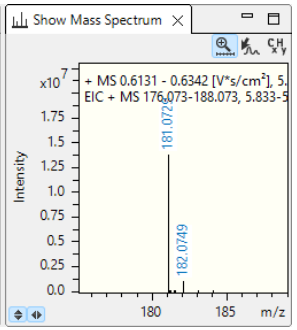
TASQ 2026B: Show Heat Map: Point and Click for Manual Integration in two dimensions simultaneously

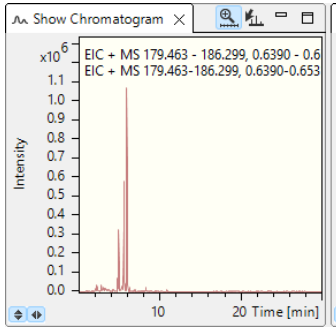


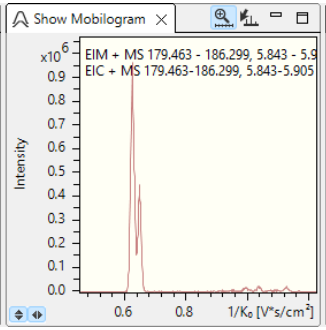












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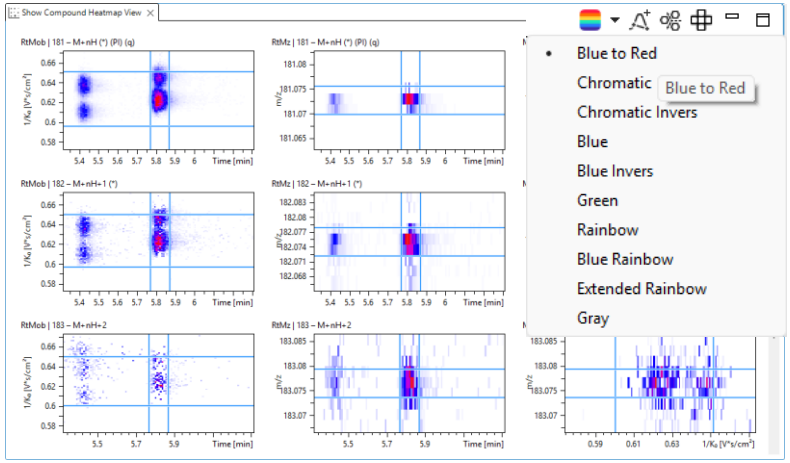
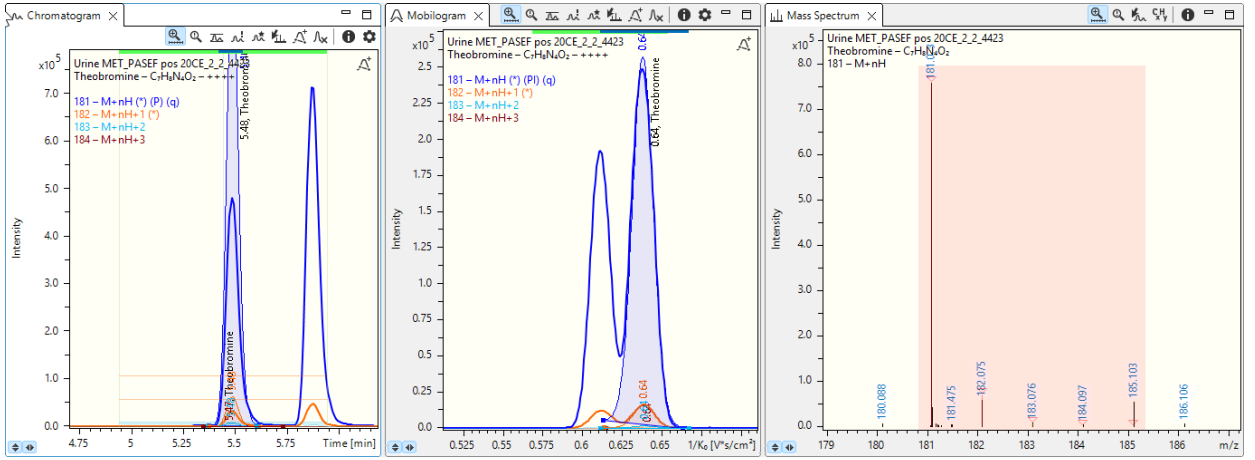
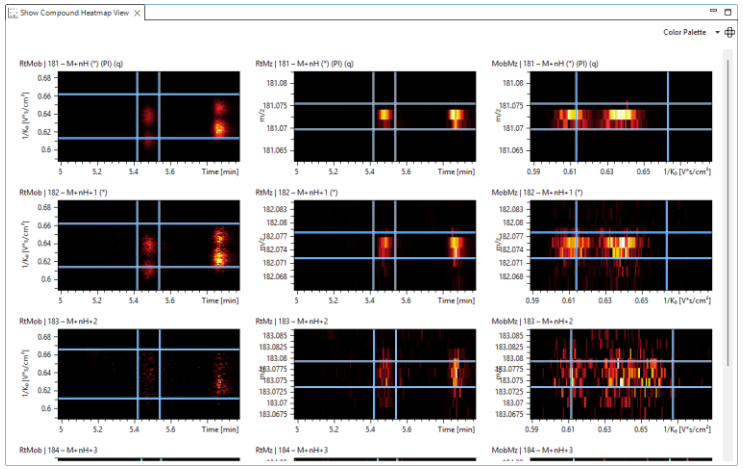
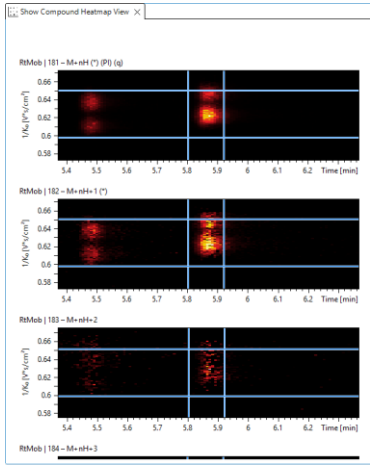
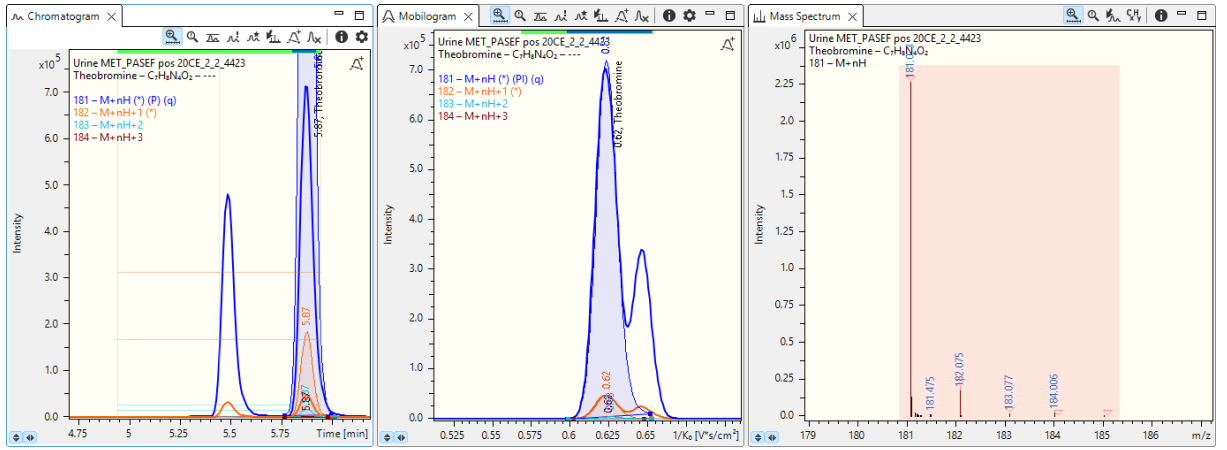
TASQ 2026B: Show Compound Heat Map: Color Palette and Manual Integration available – Update Determination











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TASQ 2026B: Show Compound Heat Map: Manual Integration

- Manual integration in the Show Compound Heat Map view is a process in two steps
- First the user selects a range then he asks to perform the manual integration
- Either the user selects a range be drag and drop of a rubber band
- Or the user activates segment detection and the user clicks on a peak in the heat map
- When a segment was detected the user can change the threshold for the segment selection with [SHIFT] Mouse Wheel and enlarge or shrink the detected segment
- By pressing the manual integration toolbar icon or the [X] key manual integration will be performed.
- The toolbar is shown outside the Show Compound Heat Map view space

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TASQ 2026B: Show Compound Heat Map Views – Manual Integration

- Currently no replay of manual integration is availble on process batch if manual integration was done in Show Compound Heat Map

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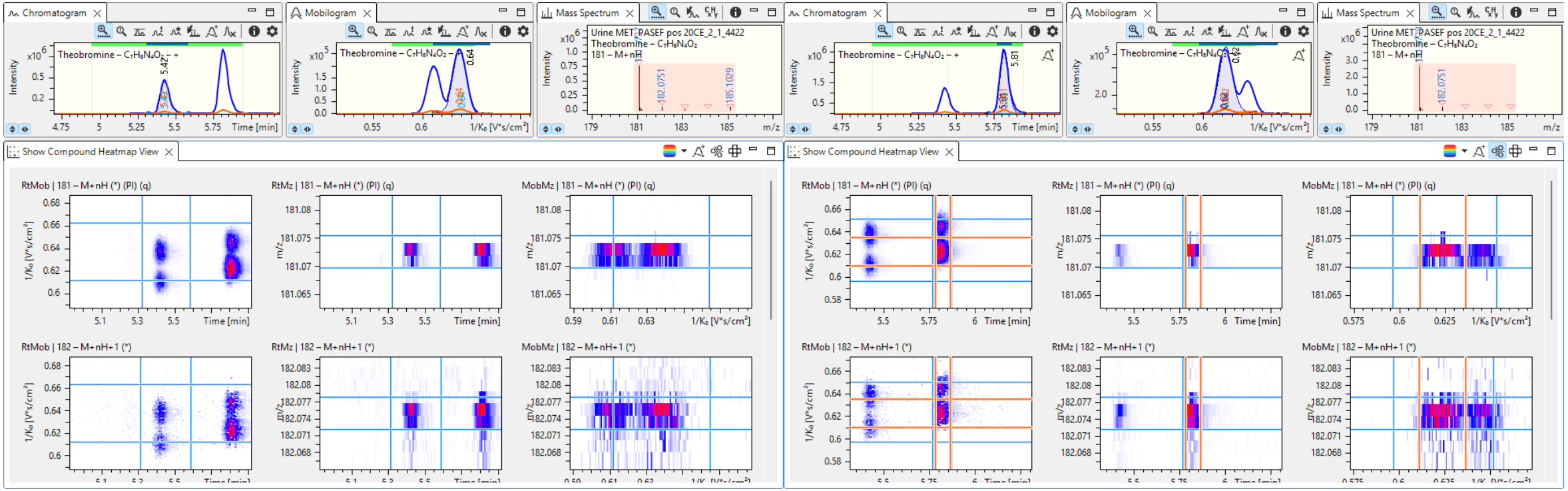
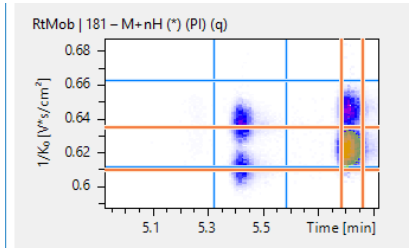
TASQ 2026B: Show Compound Heat Map: Manual Integration by Segment Selection





- Select region or click on visible peak
- With [SHIFT] Mouse Wheel enlarge or shrink the segment
- With [x] invoke manual integration

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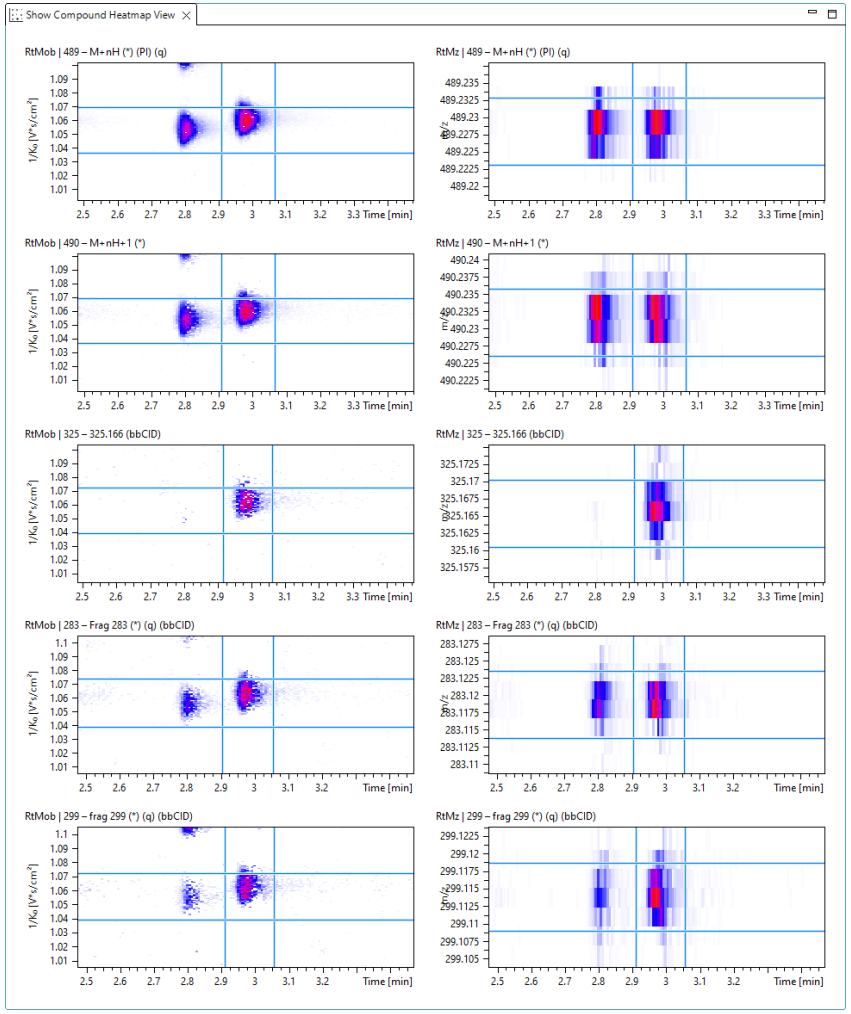
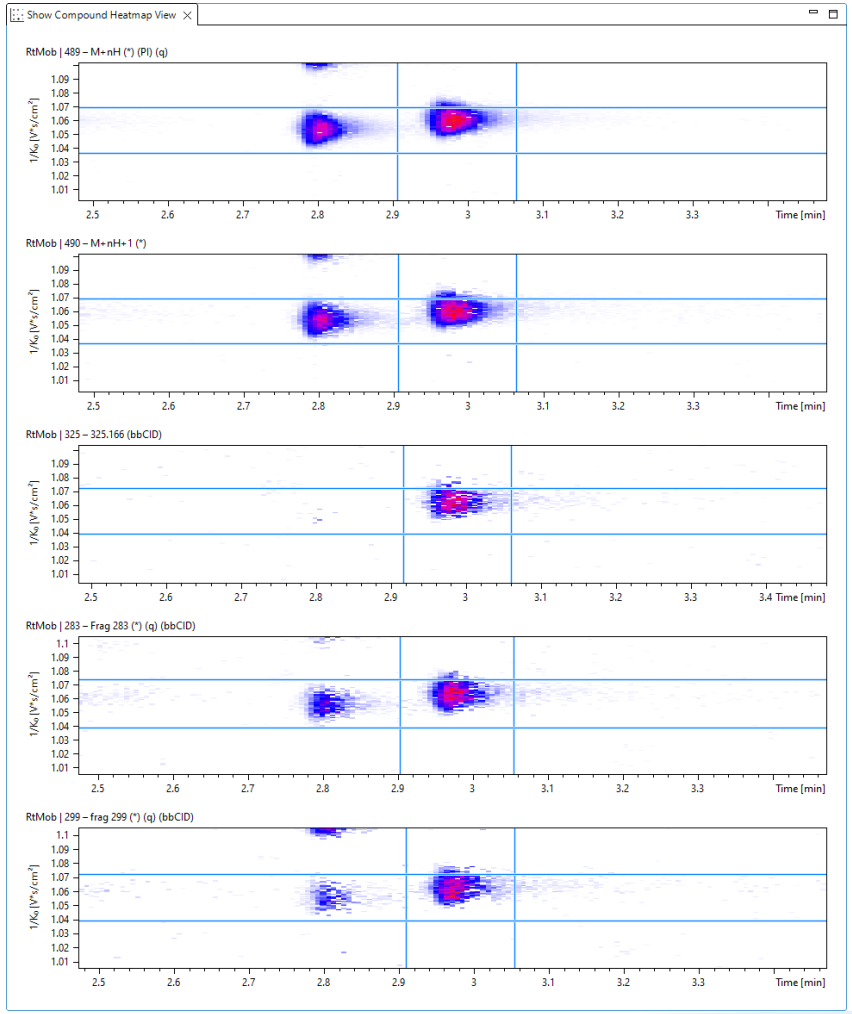
TASQ 2026B: Show Compound Heat Map

- Option to specify which columns shall be visible





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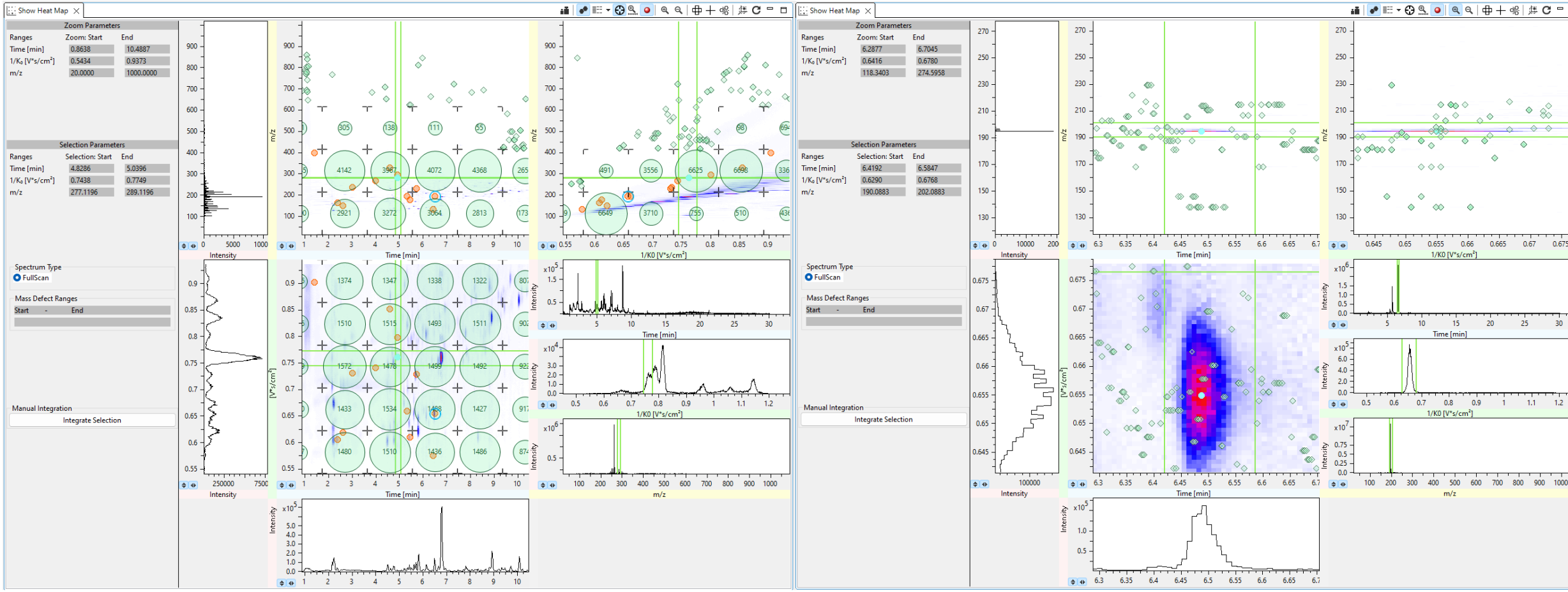
TASQ 2026B: Show Heat Map: Overlay MS/MS Events



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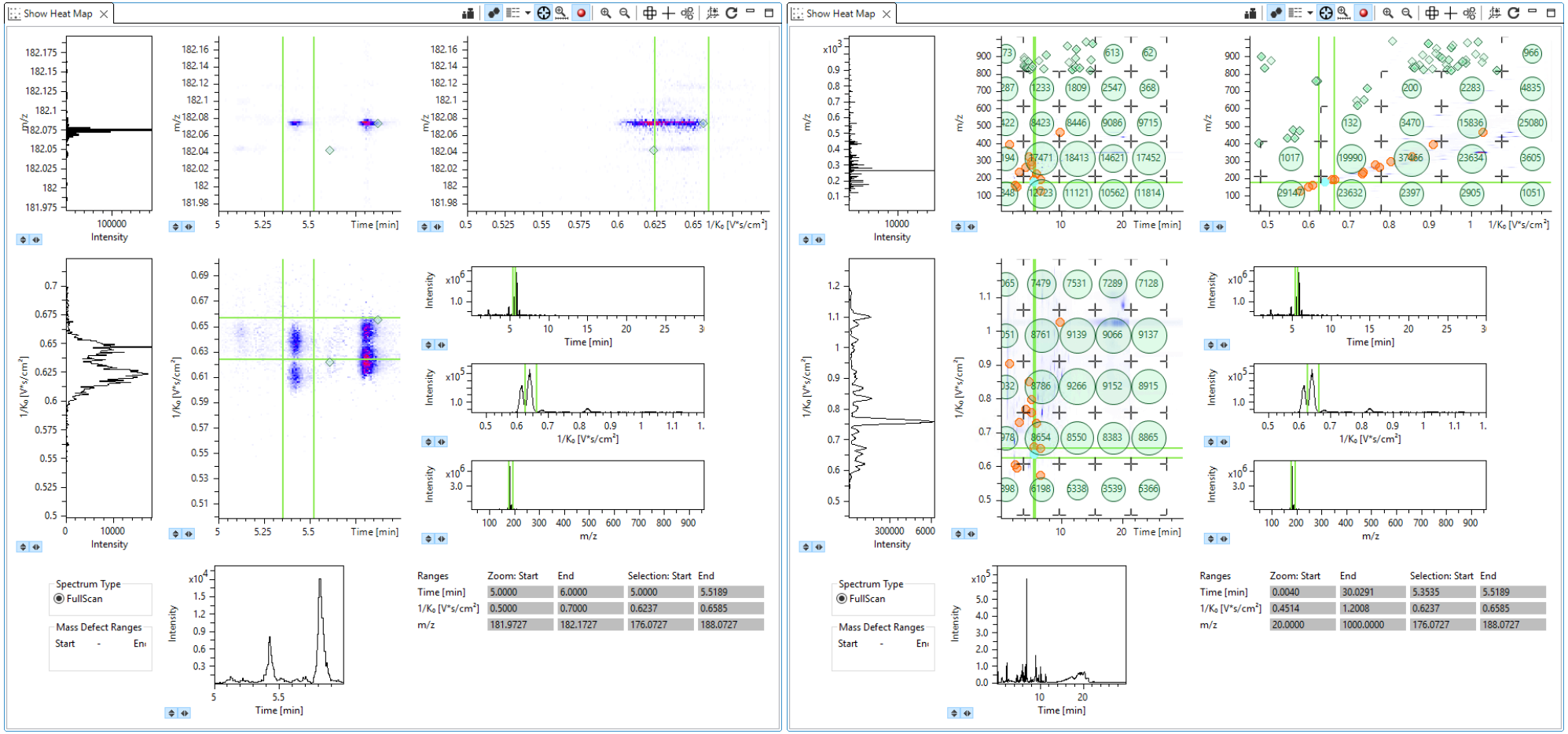
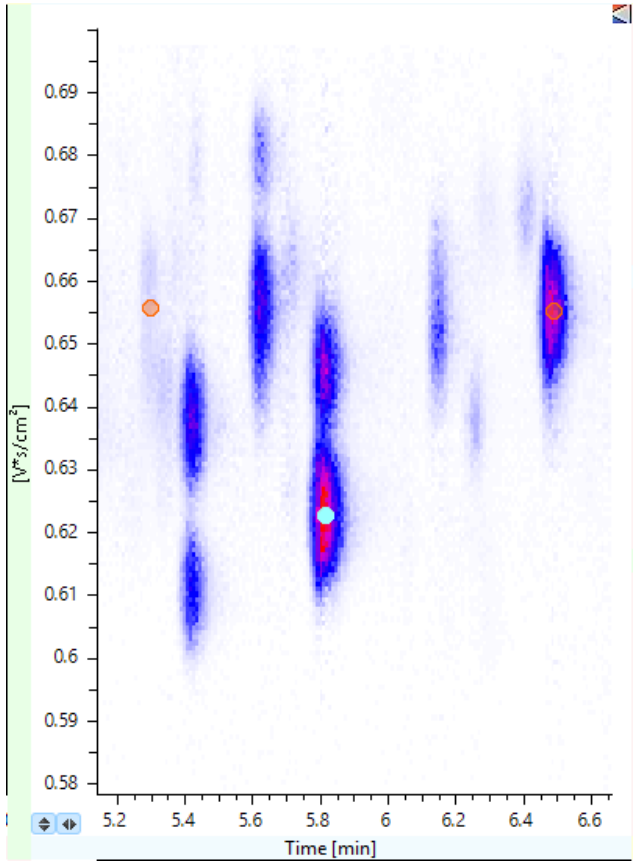
TASQ 2026B: Overlay MS/MS Events on Heat Map

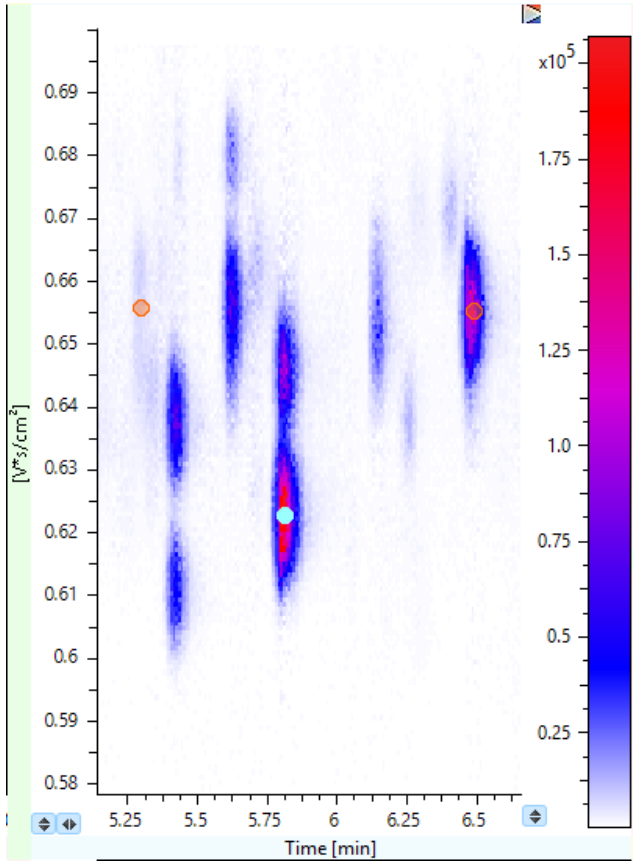
- Overlay MS/MS event which are in visible cuboid
- If too many: show statistical information

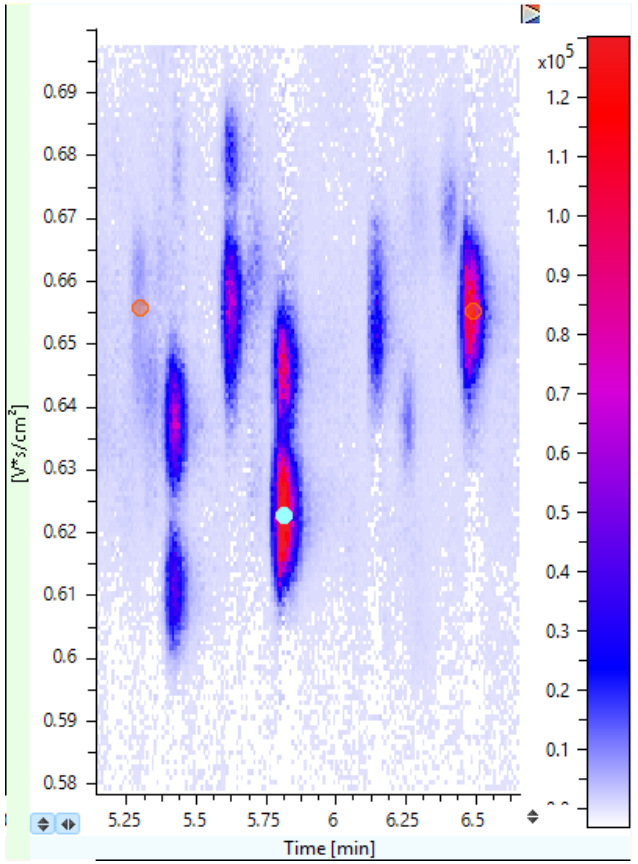


TASQ 2026B: Heat Map View – Show/Hide Color Scale

- Show or hide color scale to change the visible data points and color of data points based by intensity







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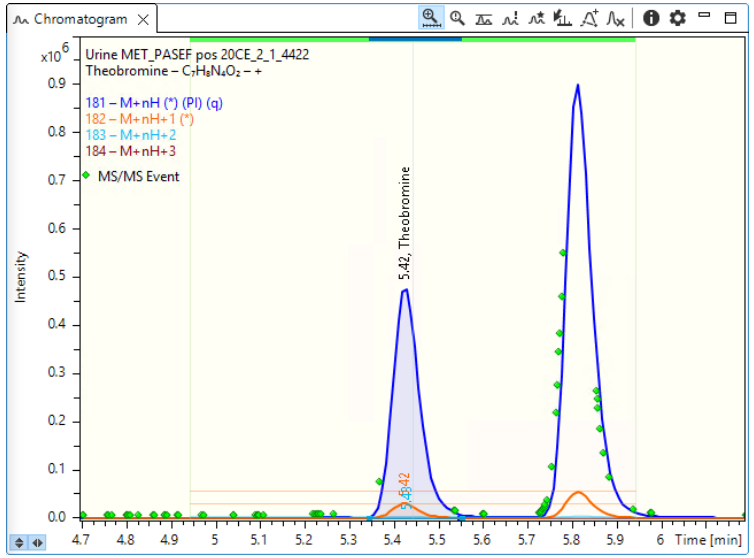
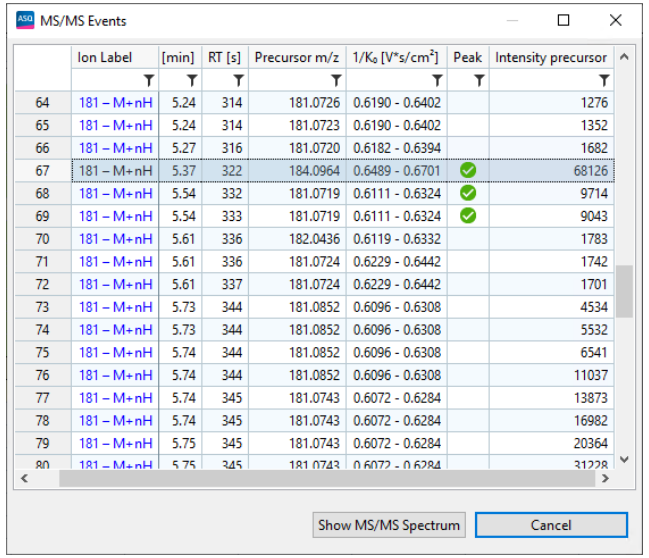
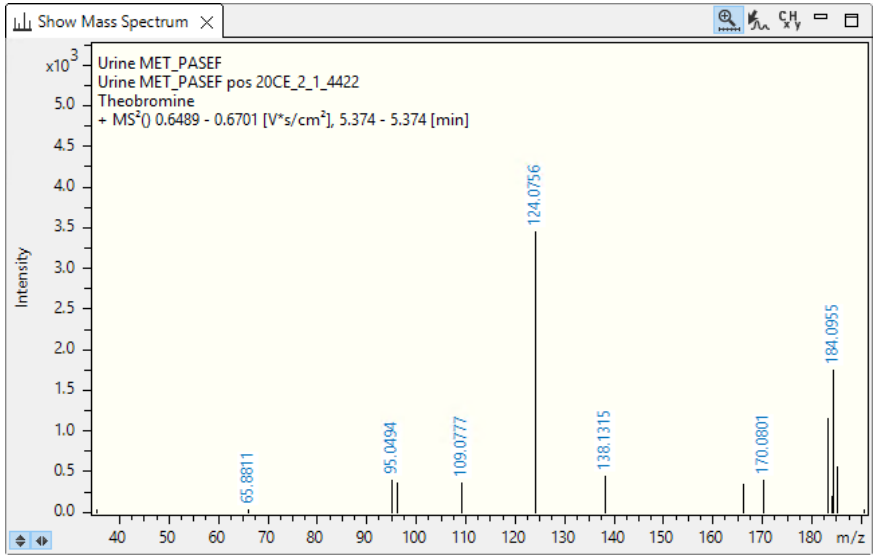
TASQ 2026B: MS/MS Events: Show MS/MS Spectrum







- Show MS/MS spectrum in Show Mass Spectrum view
- Proceed to SmartFormula view to interpret dominant MS/MS Fragments and add to TASQ processing method
- Planned: average multiple MS/MS events

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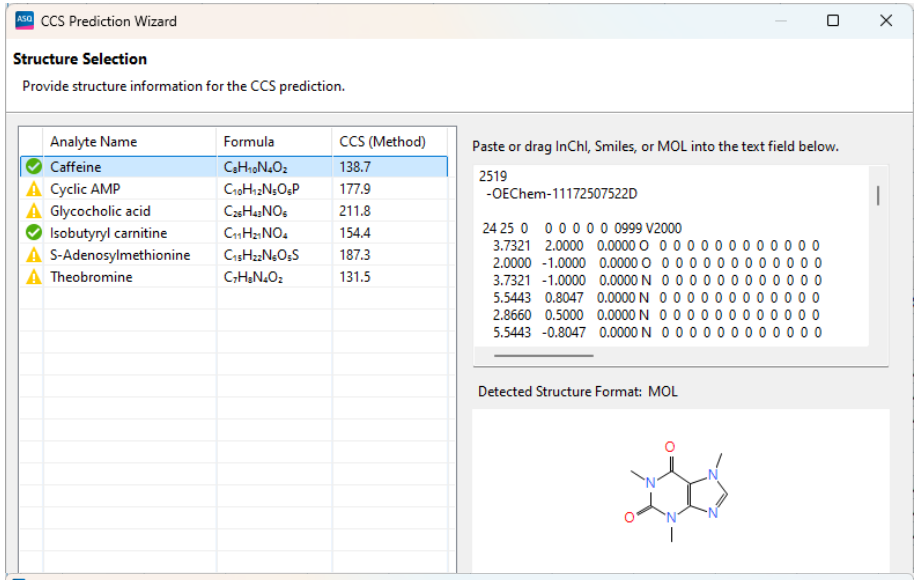
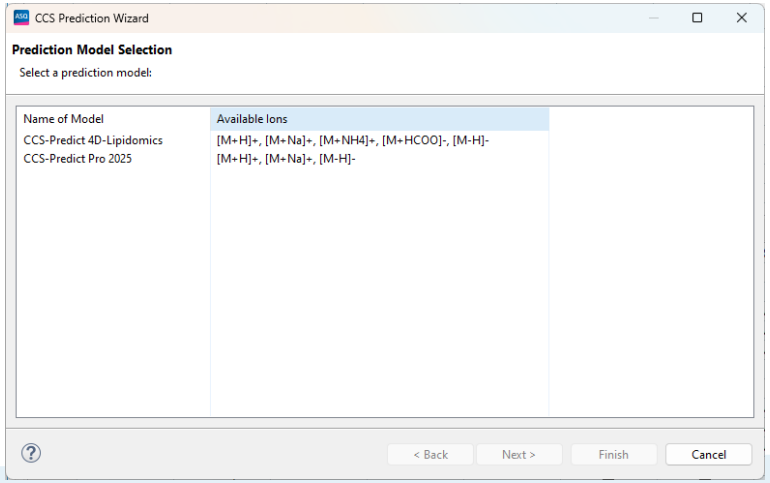
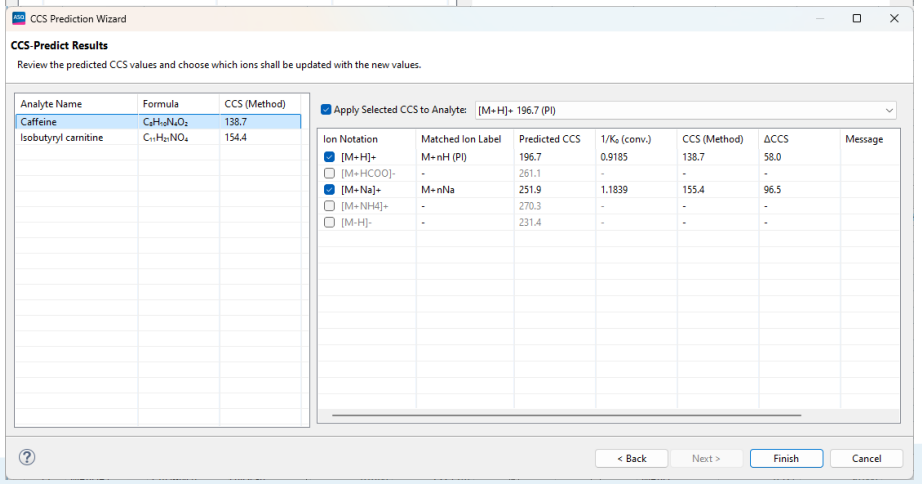
TASQ 2026B: CCS Predict for Multiple Analytes at Once

- Select multiple analytes in TASQ method and choose „Predict CCS values…“ from context menu
- Select prediction model
- Drag & Drop structure information if no structure is available
- Review prediction results and select values to be transferred to TASQ method







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TASQ 2026B: Miscellaneous

- Enable weighting with variance of signal for quantification
- Method Matcher new option to show only analytes which are present on both sides but do have different settings
- Maintenance of Statistics Table and Statistics Graph to show newly added numerical properties of determinations
- Navigate previously reviewed batches by pressing [ALT] ←, [ALT] →
- Enable Enhanced Linear Mobility calibration
  - User can specifiy in TASQ processing method which model shall be used

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TASQ 2026B: Miscellaneous

- Introduce block selection mode in nat based tables
- Switch between row selection and block selection with [CTRL-Left] S

Analysis Results

	Analyte	Formula	MRSQC	CCS Score	CCS [Å²]	ΔCCS [%]	1/K₀ [V*s/cm²]	Δm/z [mDa]	ΔRT [min]	mSigma
1	1,3-Dimethylur...	$C_7H_8N_4O_3$		++	141.26	-0.17	0.6601	-0.06	-0.02	4.9
2	1-Methyladen...	$C_{11}H_{15}N_5O_4$		++	159.87	0.06	0.7614	-0.03	-0.03	16.7
3	4-Hydroxyindole	C_8H_7NO		++	126.81	0.09	0.5759	0.44	-0.02	13.4
4	7-Methylguani...	$C_6H_7N_5O$		++	131.23	-0.13	0.6062	0.86	0.02	8.1
5	7-Methylguan...	$C_{11}H_{15}N_5O_5$		++	167.36	-0.12	0.7990	-0.10	-0.03	13.8
6	Adenosine	$C_{10}H_{13}N_5O_4$		++	156.04	-0.08	0.7414	-0.55	-0.06	5.0
7	Biopterin	$C_9H_{11}N_5O_3$		++	154.84	0.05	0.7314	-0.25	-0.04	13.1
8	Caffeine	$C_8H_{10}N_4O_2$		++	140.25	-0.03	0.6550	0.62	-0.02	14.3
9	Cyclic AMP	$C_{10}H_{12}N_5O_6P$		++	177.91	-0.00	0.8530	-0.01	-0.03	4.6
10	Glycocholic acid	$C_{26}H_{43}NO_6$		++	211.57	-0.11	1.0261	0.68	-0.01	11.9
11	Isobutyryl carn...	$C_{11}H_{21}NO_4$		++	154.57	0.11	0.7291	0.62	-0.02	9.0
12	S-Adenosylme...	$C_{15}H_{22}N_6O_5S$		++	187.01	-0.14	0.9027	-0.05	0.05	74.3
13	Theobromine	$C_7H_8N_4O_2$		++	131.36	-0.11	0.6105	0.55	-0.02	6.5
14	Xanthine	$C_5H_4N_4O_2$		++	135.00	-0.19	0.6198	0.12	-0.01	11.0

Analysis Results

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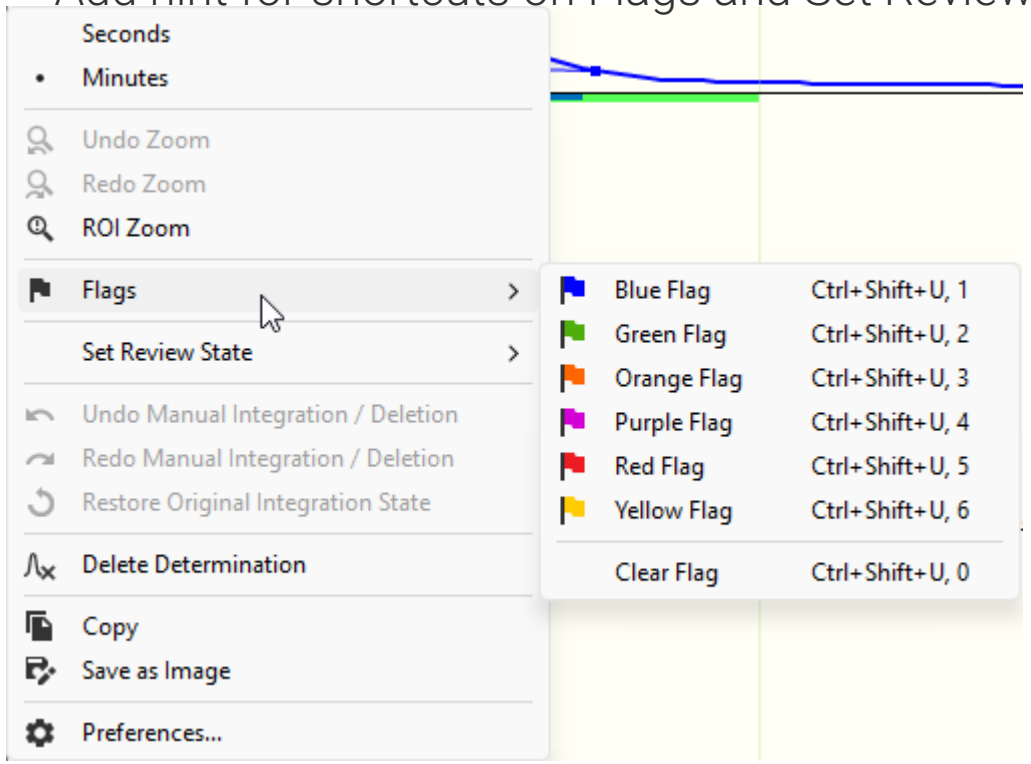
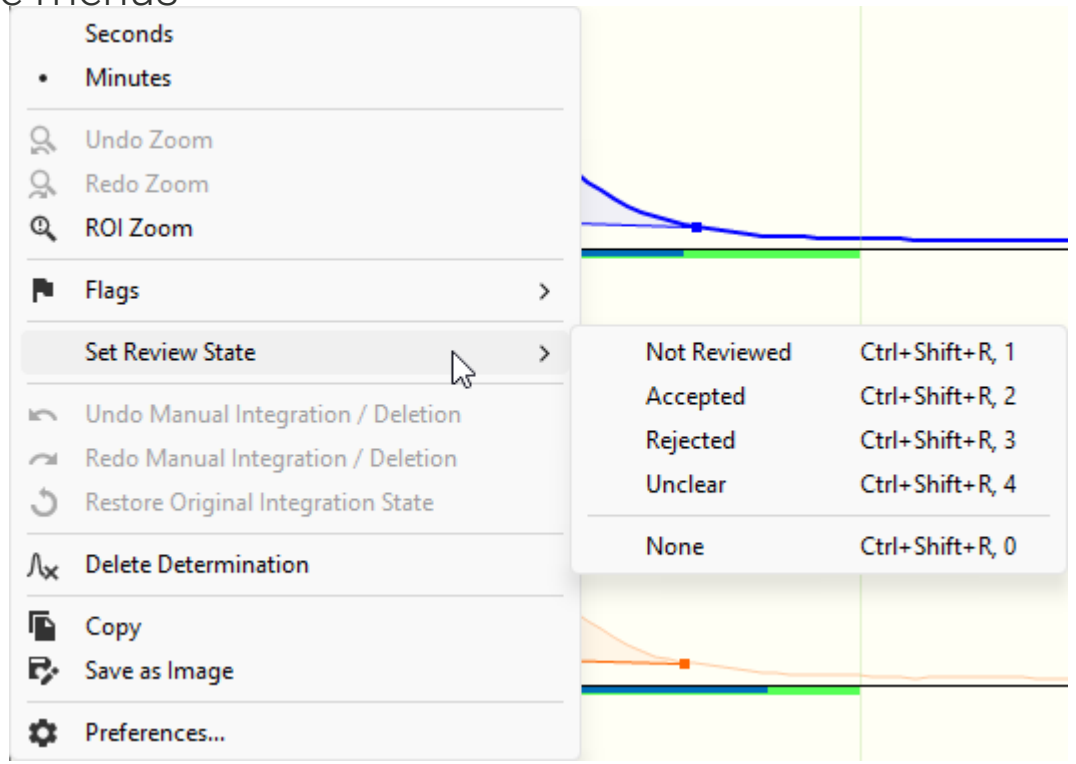
TASQ 2026B: Miscellaneous

- Set flags and review states in Chromatogram/s and Mobilogram/s view with CTRL-SHIFT F, 0..6 and CTRL-SHIFT R, 0..5
- Add hint for shortcuts on Flags and Set Review State menus





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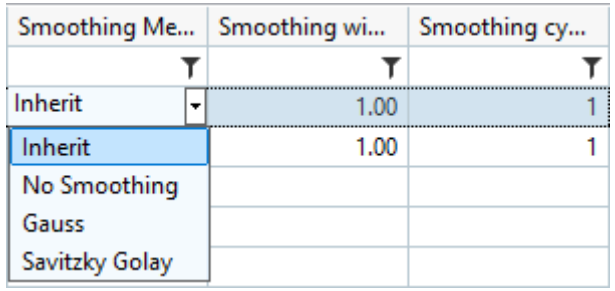
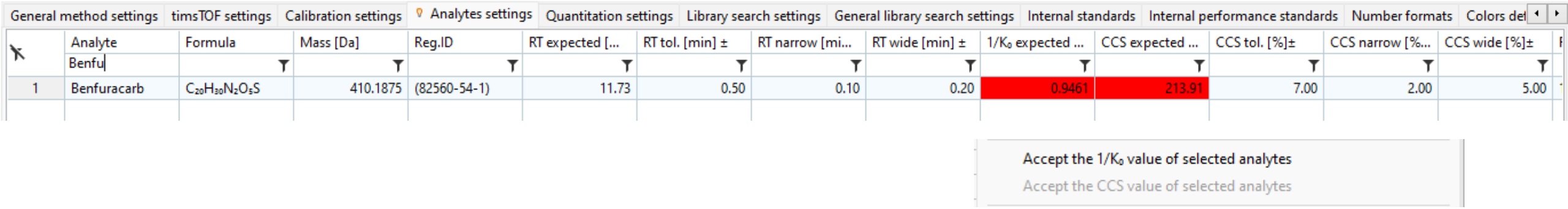
TASQ 2026B: Miscellaneous

- Enhanced specification of smoothing parameters on ion level – no smoothing – same smoothing algorigthm as specified in global settings – Gauss – Savitzky Golay



- More relaxed handling of errors in TASQ method
  - Improved editing of errorneous/conflicting 1/K0 and CCS values
- Allow processing again even if there are errors in TASQ method



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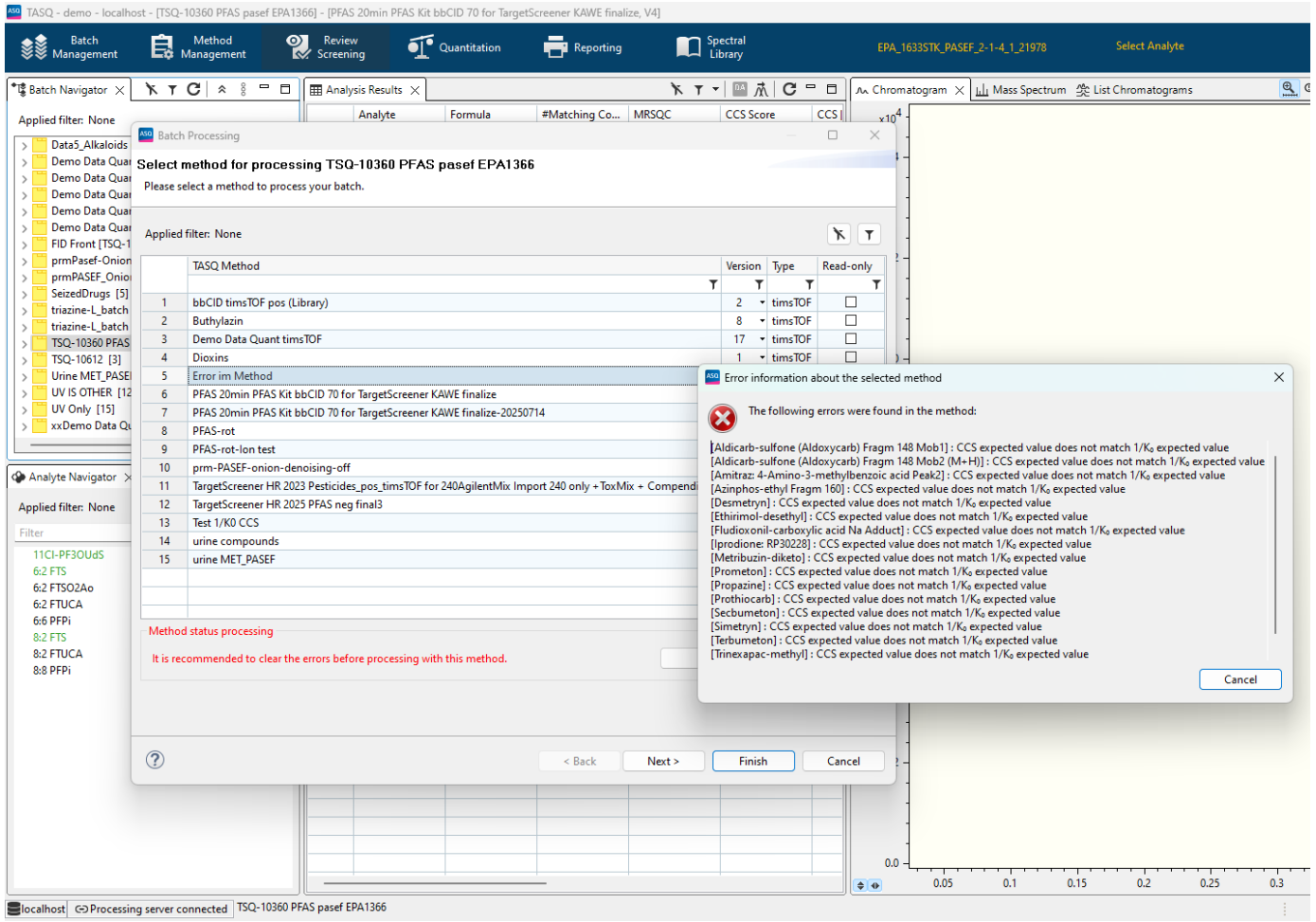
TASQ 2026B: Miscellaneous

- Let the user process data even if there are errors or bad settings in method



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TASQ 2026B: Miscellaneous

- Extend TASQ processing method by import of tsv file.
  - Ignore duplicate analytes
  - In future merge information of duplicates
- Evaluation rule: false positive – consider chromatograms of mandatory ions to reduce number of false positive flags
- Optimize chromatogram: reduce 1/K0 range in case of broad mobility peaks to increase specifity
- Allow copy & paste of analyte within a TASQ processing method
- Be more relaxed on processing over segment borders – do not stop if next segement does not contain spectra
- For DART data show temperature profile in List Chromatograms view. More important requirement seems to be show intensity vs temperature (Thermo desorption plot)

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TASQ 2026B: Extend TASQ Processing Method with Analytes

5	13C3-PFHxS	$C_3{}^{13}C_3HF_{13}O_3S$	402.9539		8.02
6	13C4-PFBA	$^{13}C_4HF_7O_2$	217.9999		4.88
7	13C4-PFHpA	$C_3{}^{13}C_4HF_{13}O_2$	367.9903		7.97
8	13C5-PFHxA	$C^{13}C_5HF_{11}O_2$	318.9969		6.93
9	13C5-PFPeA	$^{13}C_5HF_9O_2$	269.0001		5.88
10	13C6-PFDA	$C_4{}^{13}C_6HF_{19}O_2$	519.9874		10.45
11	13C7-PFUnA	$C_4{}^{13}C_7HF_{21}O_2$	570.9876		11.05
12	13C8-PFO				8.88
13	13C9-PFN				8.73
14	3,6-OPFH				6.80
15	3,6-OPFH				6.80
16	4:2 FTS				6.90
17	6:2 FTS				8.92
18	8:2 FTS				10.50
19	9CI-PF3O				10.20
20	ADONA				8.12
21	ADONA F				8.12
22	EtFOSA				12.70
23	EtFOSAA				11.20
24	EtFOSE				2.50
25	FHpPA				10.03
26	FOSA				11.10

Set Tags to Selected Analytes

Add Analyte

Add Analytes from File...

Remove Analytes DEL

Paste Analytes

Copy selected Analytes

Add Missing Ion Ratios

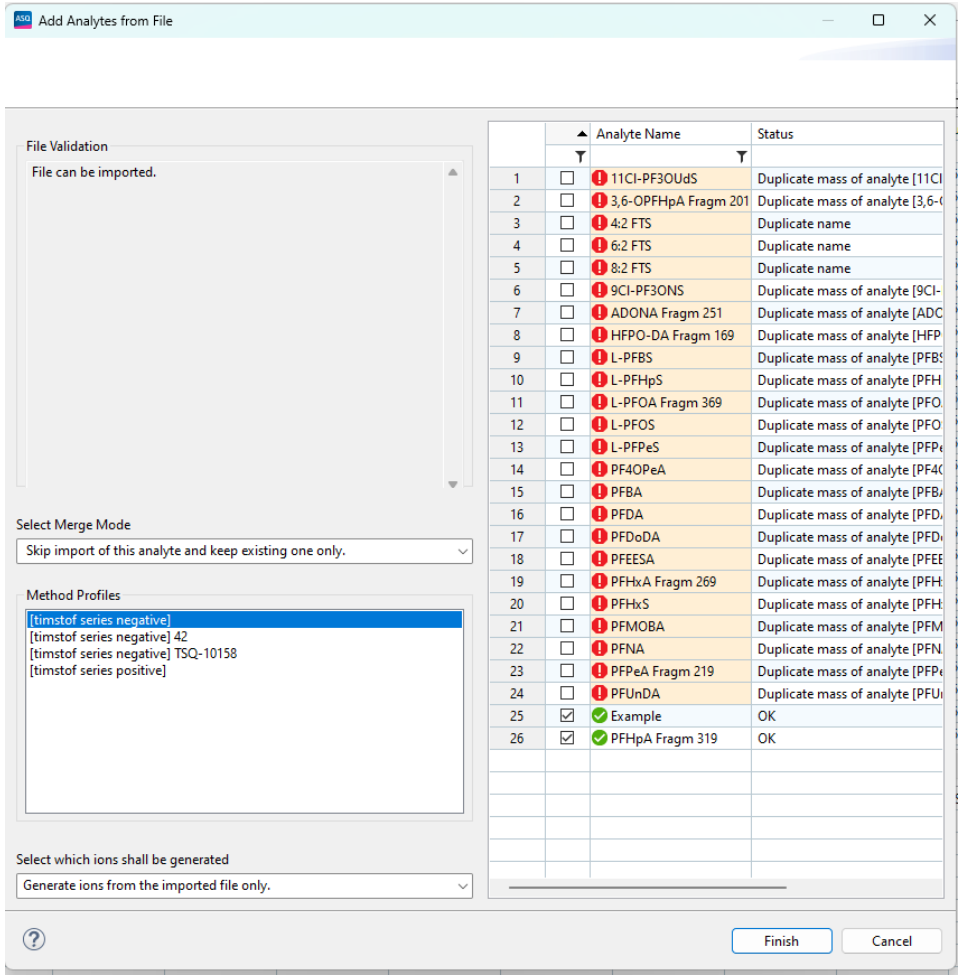
Change Retention Times Offset...

Delete Sigma and Tau Values of all Analytes

Select Evaluation Rules

Clone Method for selected Analytes

Clone Method for Fluxomics for selected Analytes



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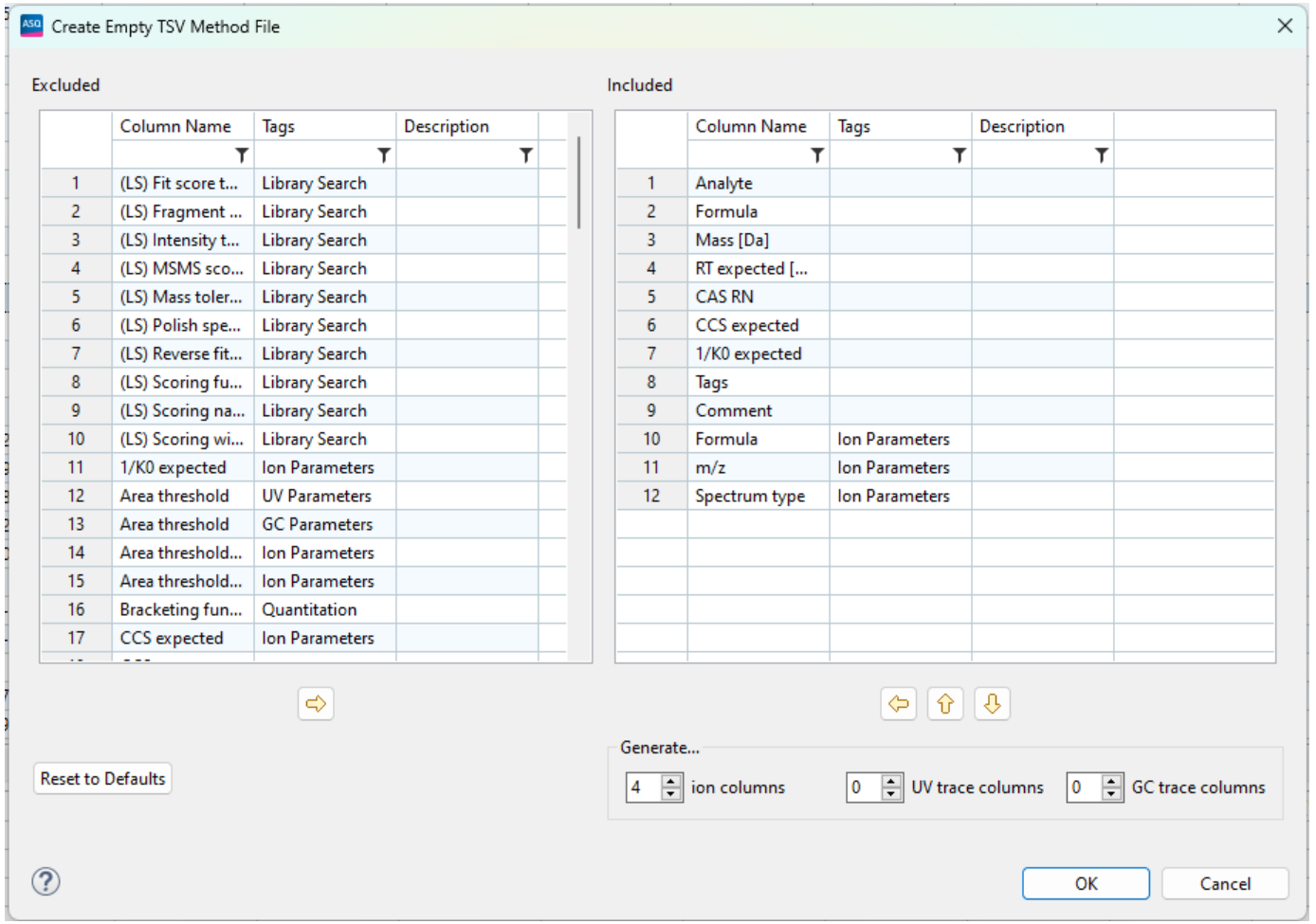
TASQ 2026B: Extended Configure Columns Dialog: Tags for Columns

- Hence there are myriads of columns tags were added to categorize columns
- Configure columns dialog can be filtered or sorted by the tags column
- Also available for creating a template tsv file to organize analyte information for generation of TASQ processing methods from file or extension of TASQ processing method by file



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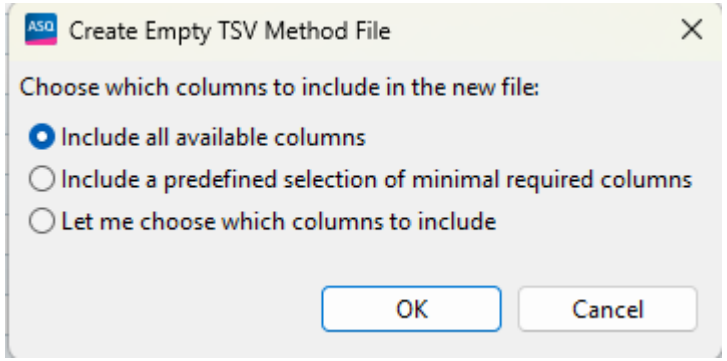
TASQ 2026B: Create Empty TSV Method File

- Creation of Empty TSV Method File is improved
- There are now three options:
  - Create an empty TSV file containg all available columns
  - Create an empty TSV file with a minimu set of columns
  - Allow user to configure the set of columns with an extended configure columns dialog



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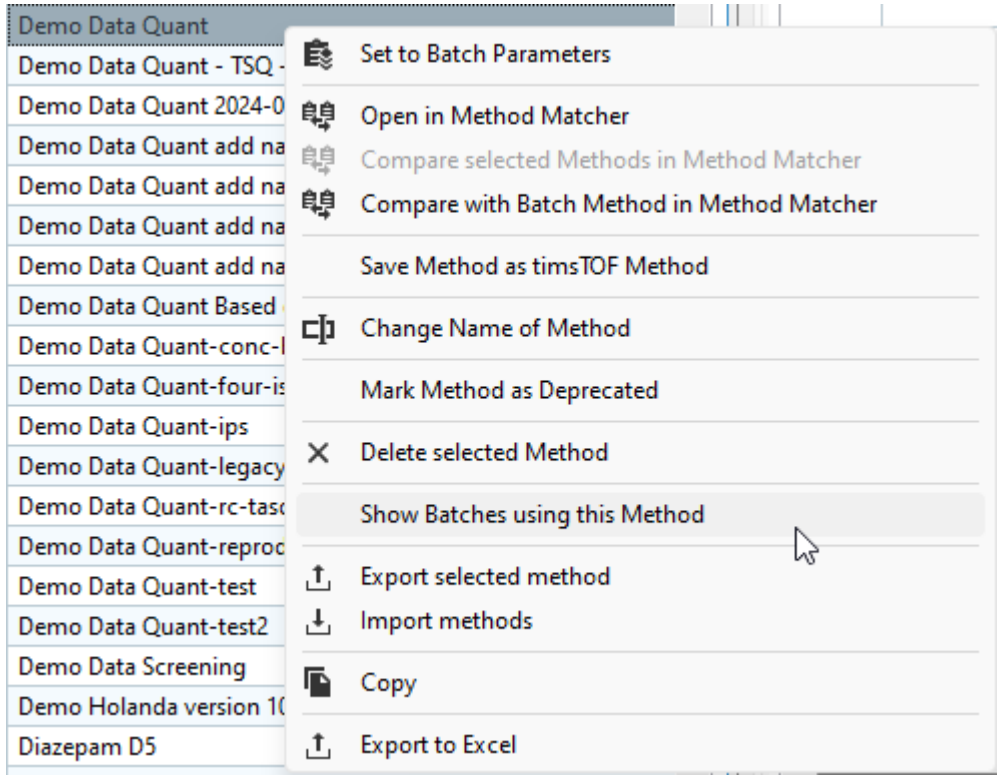
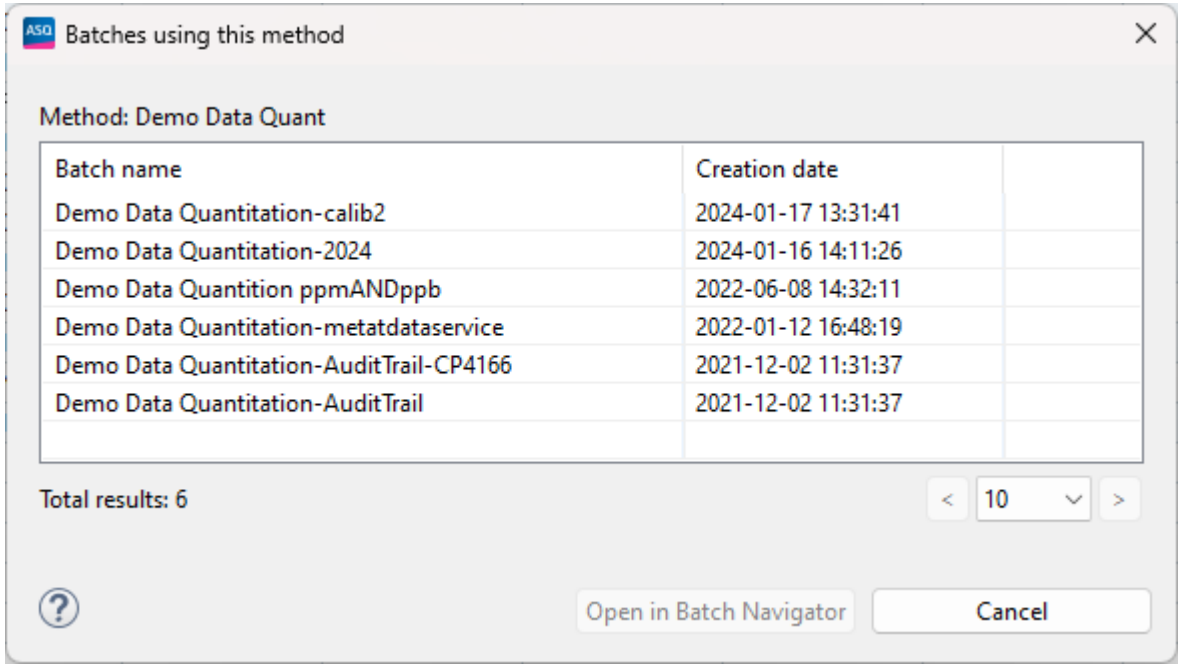
TASQ 2026B: Retrieve Batches by TASQ Method

- Retrieve a list of batches which were processed with a TASQ processing method
  - Select a batch from the result list





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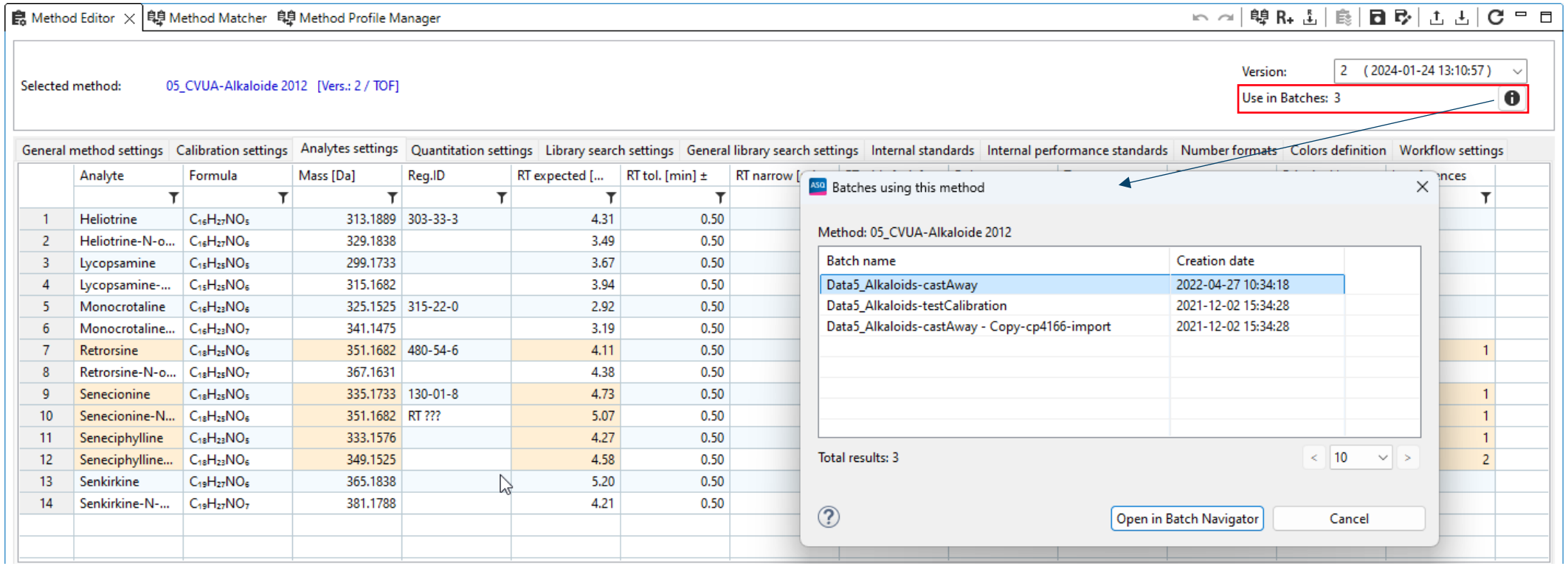
TASQ 2026B: Method Editor Give Information how many Batches were Processed with Selected Method

- Show how many batches were processed with current TASQ method
- Press Info button to get a list of batches which were processed with that method



	Analyte	Formula	Mass [Da]	Reg.ID	RT expected [...	RT tol. [min] ±
1	Heliotrine	$C_{16}H_{27}NO_5$	313.1889	303-33-3	4.31	0.50
2	Heliotrine-N-o...	$C_{16}H_{27}NO_6$	329.1838		3.49	0.50
3	Lycopsamine	$C_{15}H_{25}NO_5$	299.1733		3.67	0.50
4	Lycopsamine-...	$C_{15}H_{25}NO_6$	315.1682		3.94	0.50
5	Monocrotaline	$C_{16}H_{23}NO_6$	325.1525	315-22-0	2.92	0.50
6	Monocrotaline...	$C_{16}H_{23}NO_7$	341.1475		3.19	0.50
7	Retrorsine	$C_{18}H_{25}NO_6$	351.1682	480-54-6	4.11	0.50
8	Retrorsine-N-o...	$C_{18}H_{25}NO_7$	367.1631		4.38	0.50
9	Senecionine	$C_{18}H_{25}NO_5$	335.1733	130-01-8	4.73	0.50
10	Senecionine-N...	$C_{18}H_{25}NO_6$	351.1682	RT ???	5.07	0.50
11	Seneciphylline	$C_{18}H_{23}NO_5$	333.1576		4.27	0.50
12	Seneciphylline...	$C_{18}H_{23}NO_6$	349.1525		4.58	0.50
13	Senkirkine	$C_{19}H_{27}NO_6$	365.1838		5.20	0.50
14	Senkirkine-N-...	$C_{19}H_{27}NO_7$	381.1788		4.21	0.50

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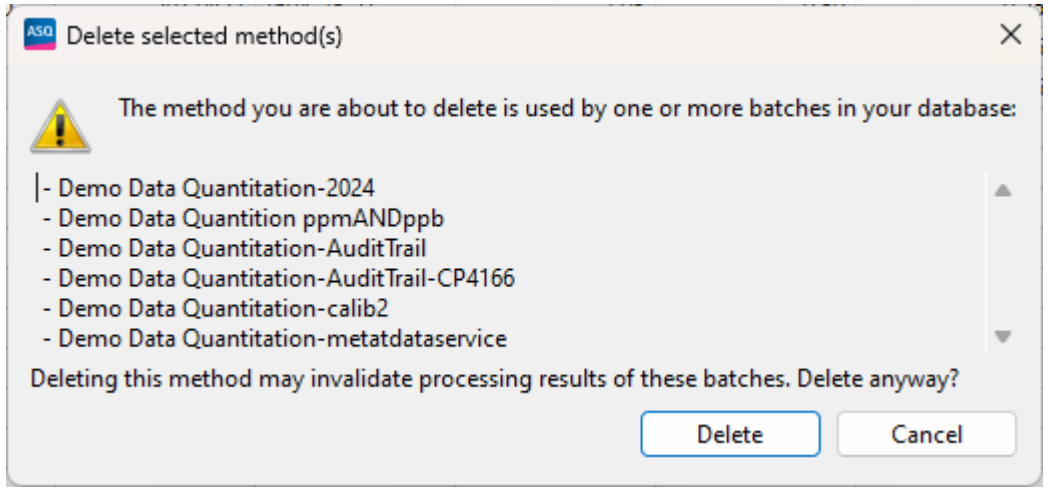
TASQ 2026B: Retrieve Batches by TASQ Method

- Delete TASQ method now checks which batches are related to this method.



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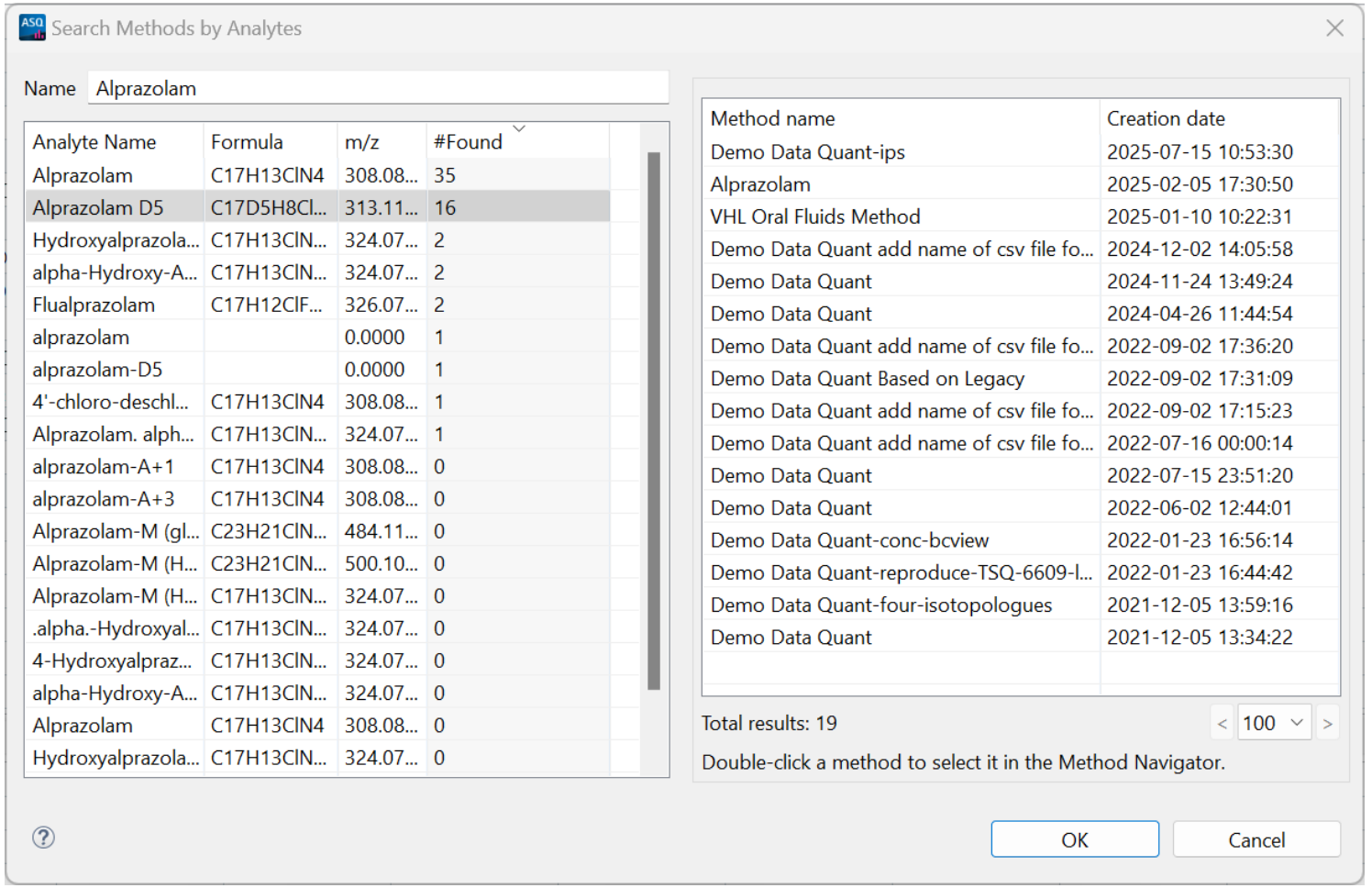
TASQ 2026B: Search for Methods which Contains Analytes

- Search for analytes
- Select analyte/s of interest
- Methods with analyte/s are listed
- Select method by double click
- **Note:** Only methods which are used for processing can be found



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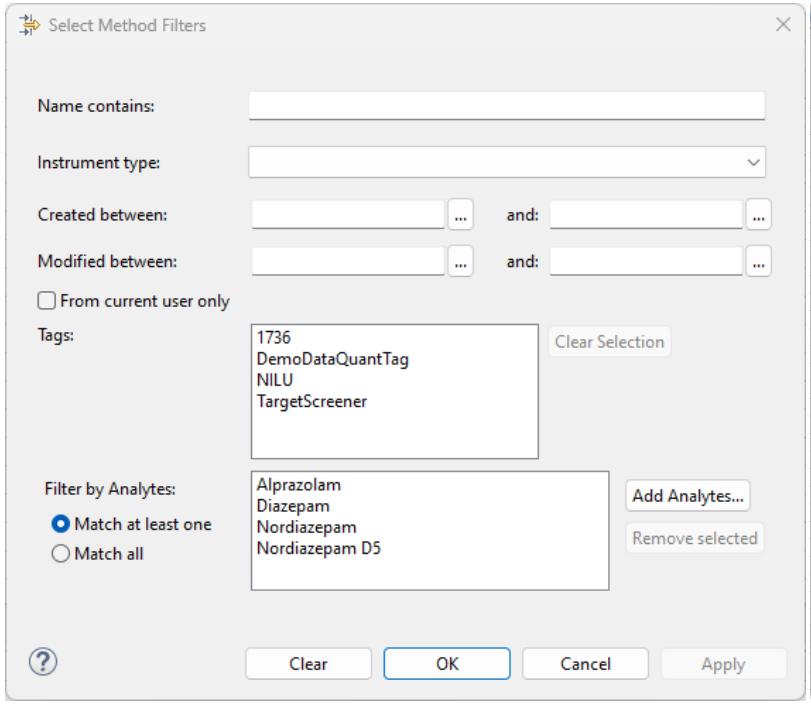
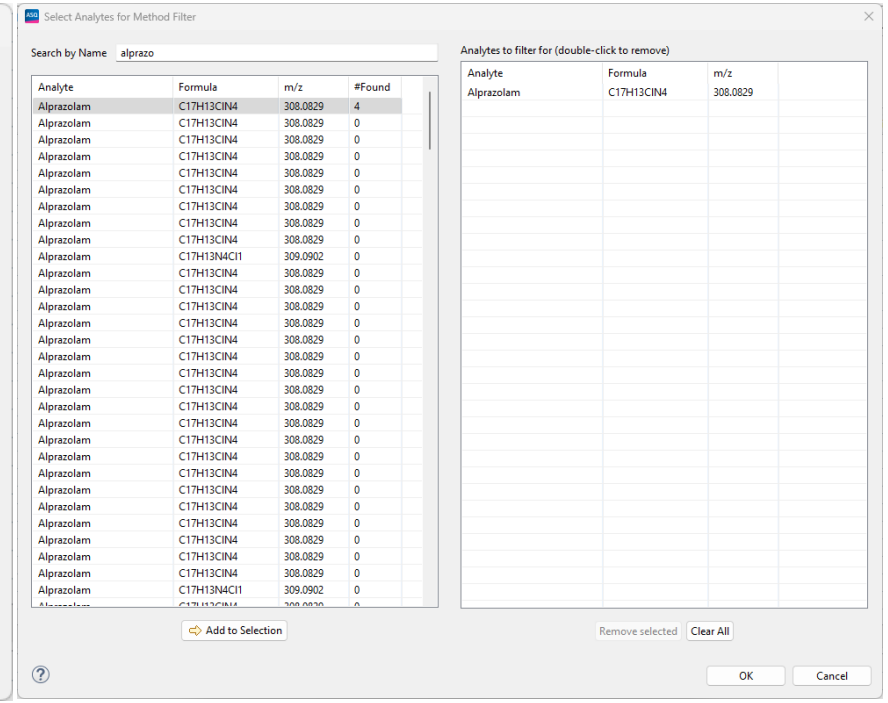
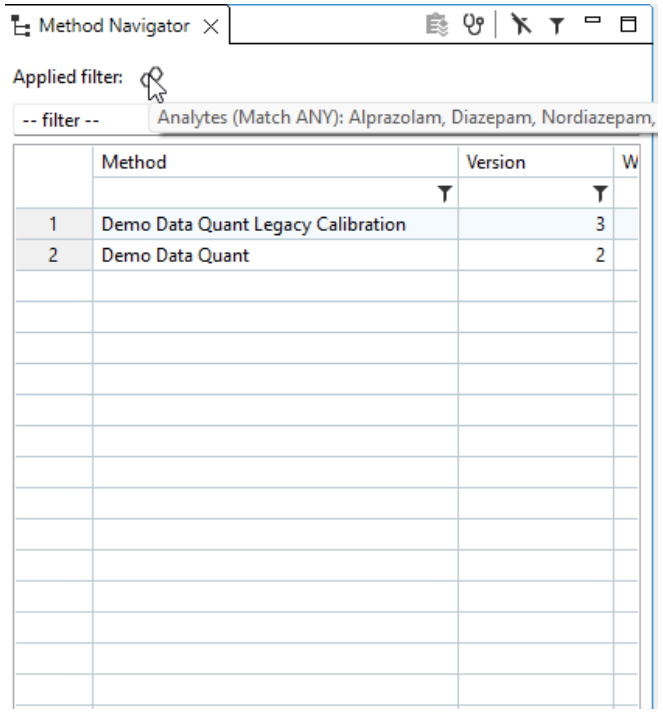
TASQ 2026B: Method Navigator – Filtering for Methods with Analytes

- Analyte filter added to method navigator to drill down methods containing analytes of interest
- Options to show methods which contains any of the selected analytes or all of them







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TASQ 2026B: Miscellaneous

- List Chromatogram view added option to manually integrate all ions or traces of same type at once
- List Chromatogram view enable manual integration of internal standards
- Apply manual integration optionally to all other chromatograms of same type

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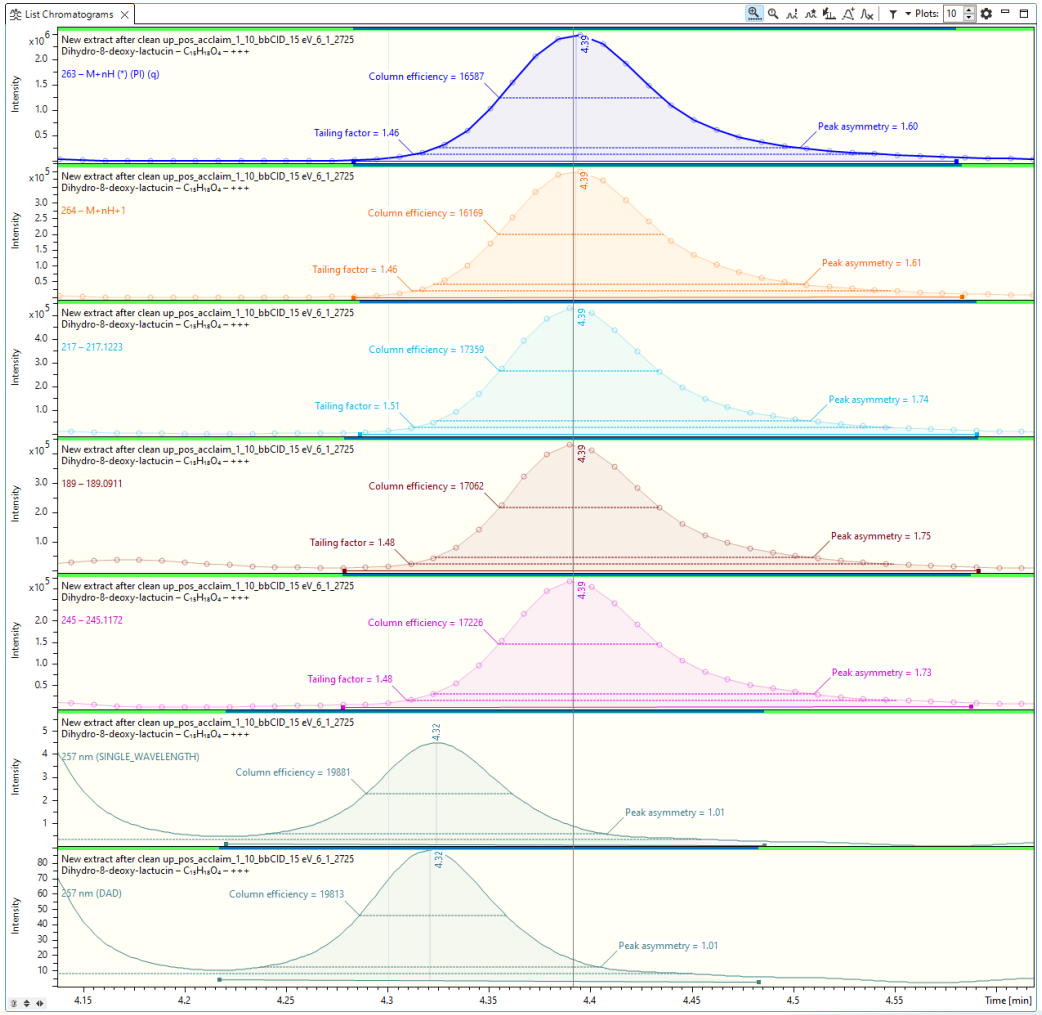
TASQ 2026B: List Chromatograms View Enhanced

- Add new option to preferences to show peak factors for MS, UV-VIS and GC peaks
- Remove square widgts on y axis as they had no function
- Add command to call preferences to context menu
- Show EIC of internal standards independently whether EICs of analyte are visible or not



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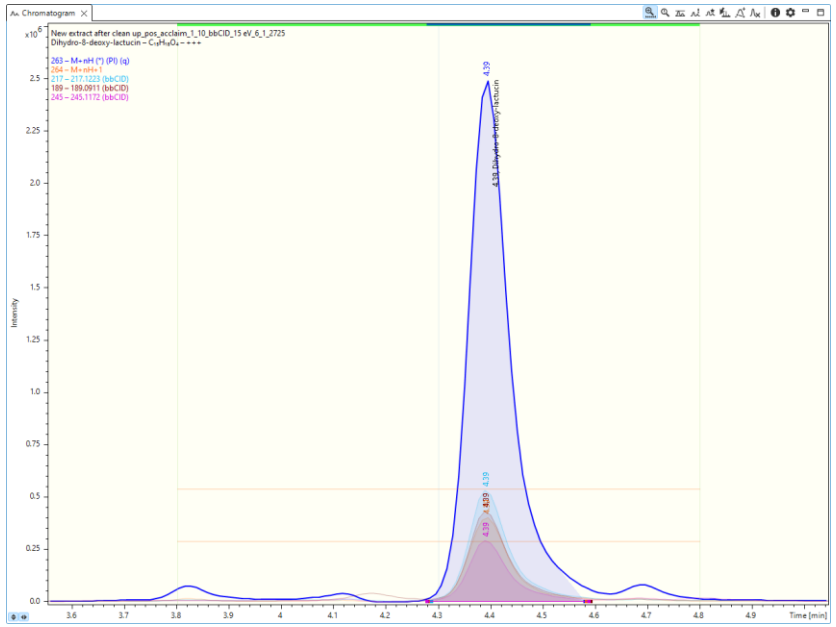
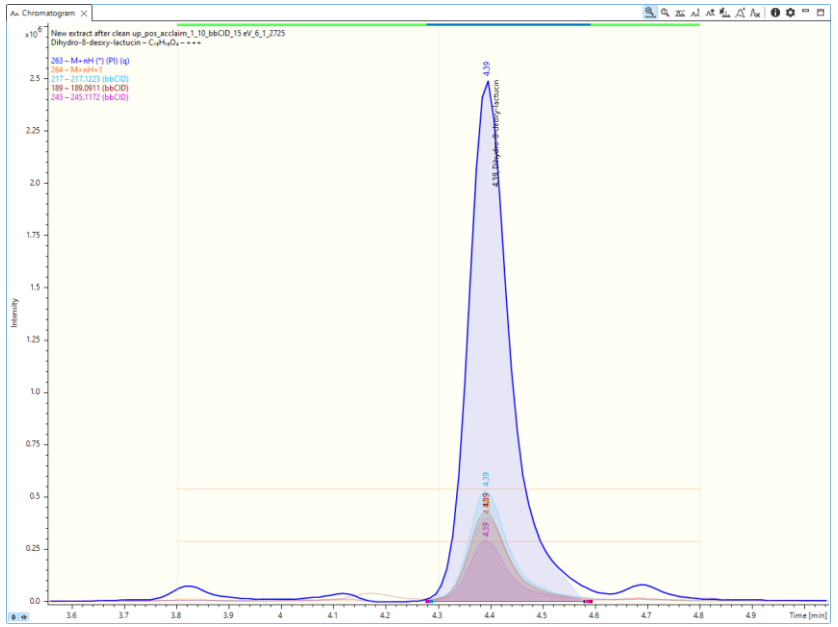
TASQ 2026B: Miscellaneous

- Use Bruker Ribbon as drop target: drag and drop .brkrar, .tasqMethod, folders with .d, or .d folders onto the Bruker Ribbon to start import of .brkrar archive, .tasqMethod or batches or extend batches.
- Option to hide upper and right border of data widget





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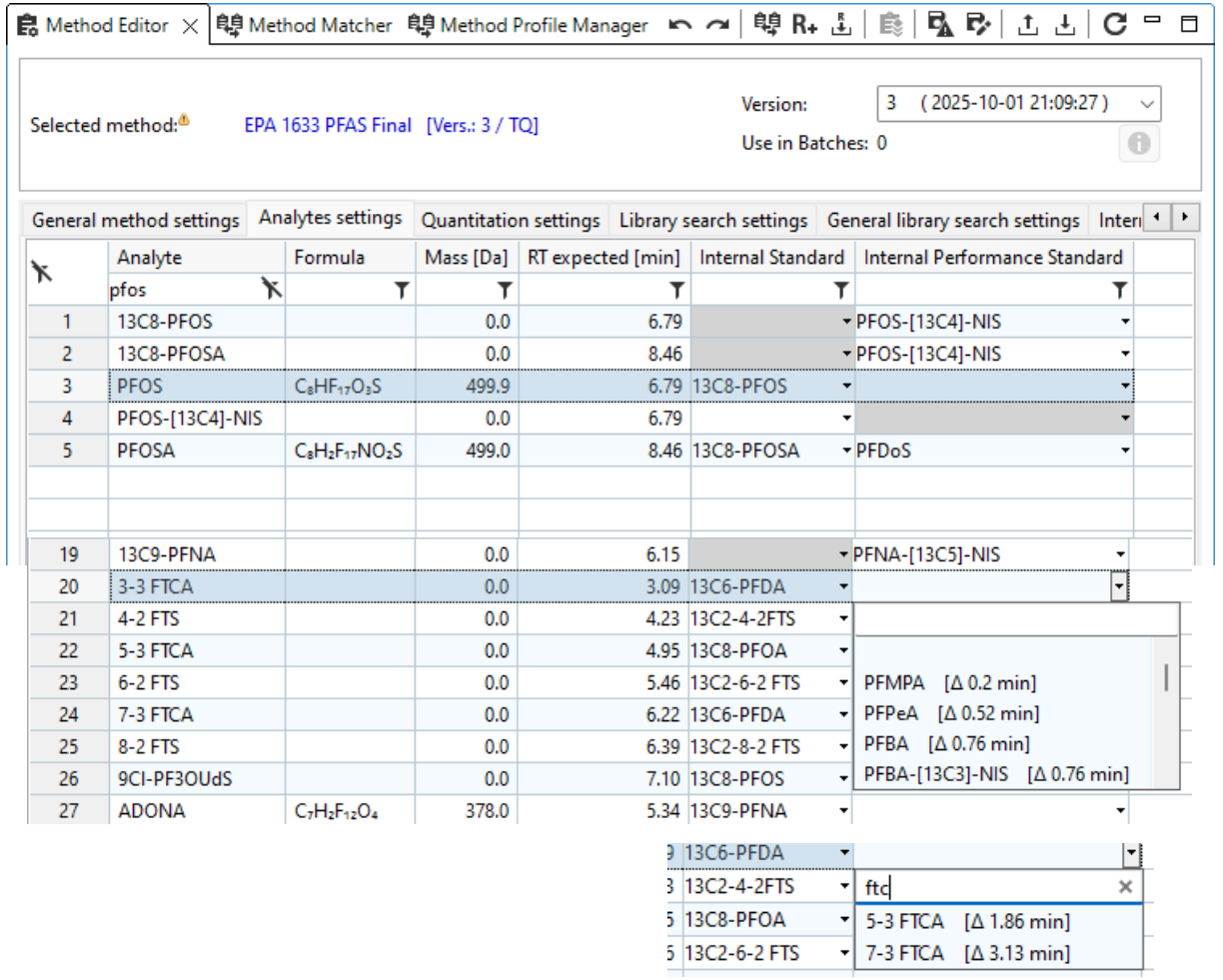
TASQ 2026B: Miscellaneous

- New columns Internal Standard and Internal Performance Standard in Analyte settings and Quantitation settings table of Method editor
- Show assigned standards
- Assign standards from combo box
- Available standards are sorted by retention time difference to selected analyte
- Analytes which are used as standard can‘t get an assignment of another analyte.
- Combo box can be filtered by entering partial name of analyte



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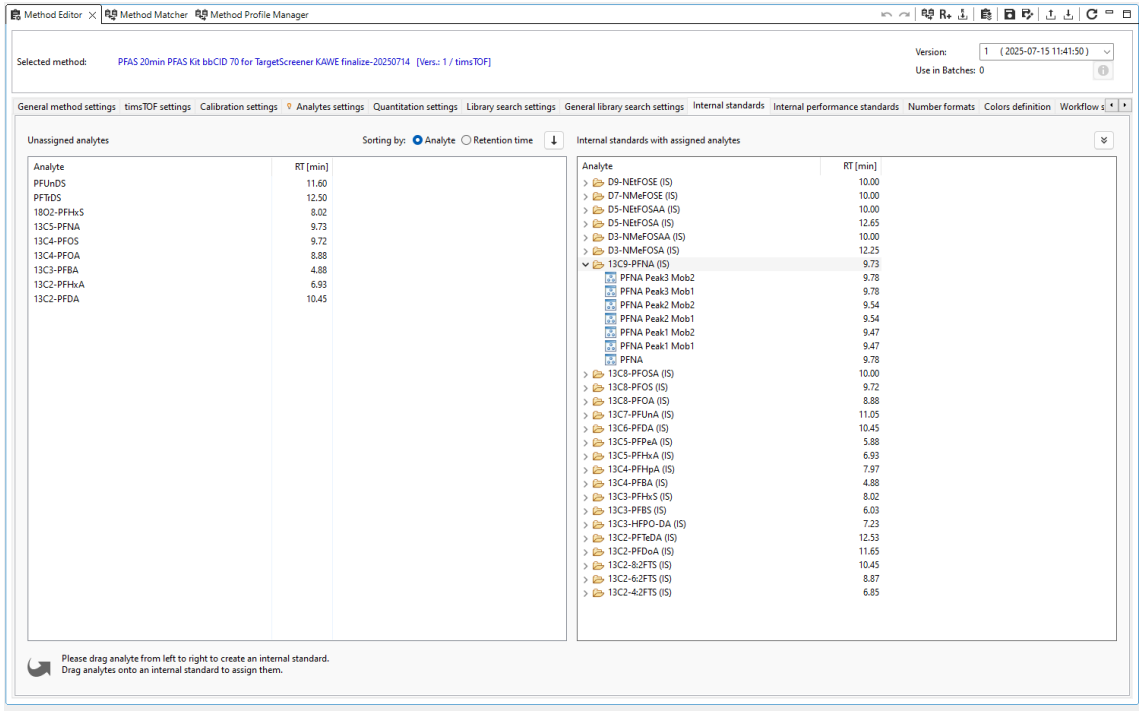
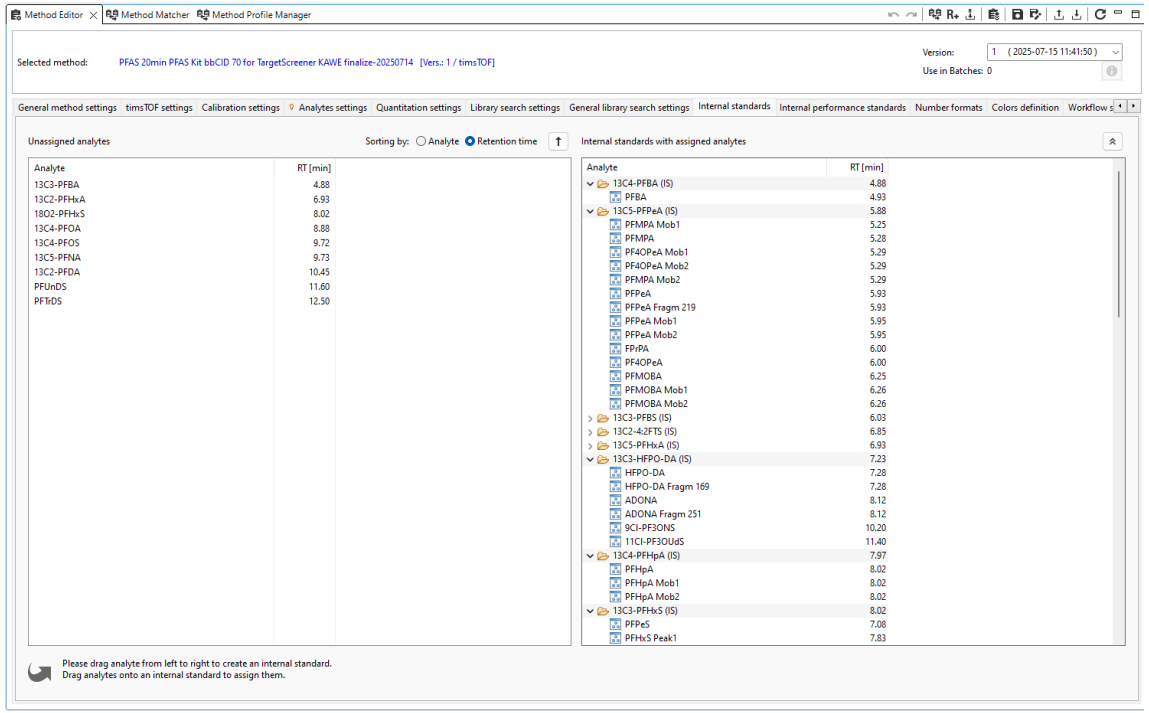
TASQ 2026B: Miscellaneous

- Internal (Performance) Standards tab in MethodEditor: Sorting of analytes by name and retention time added





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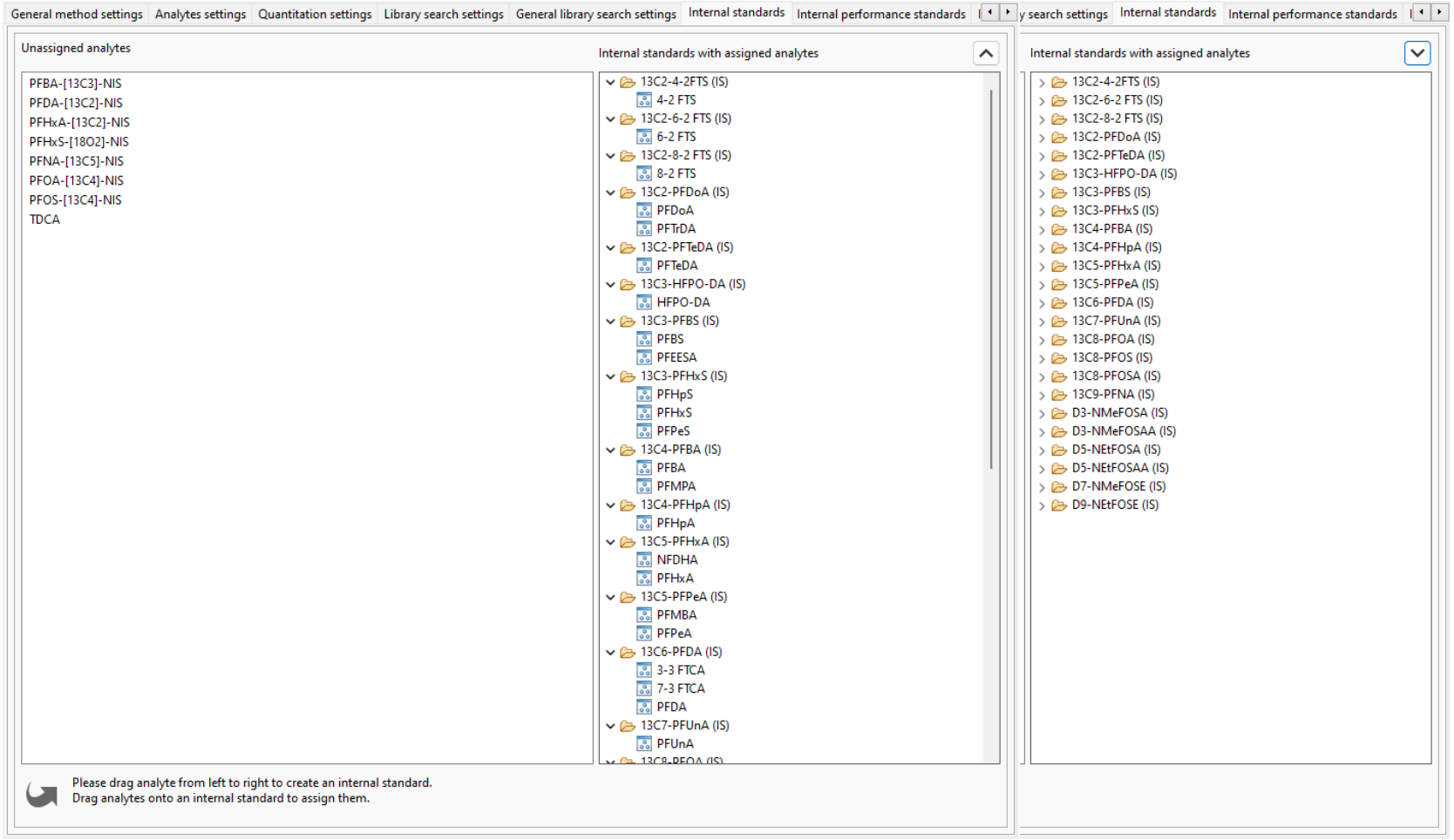
TASQ 2026B: Miscellaneous – Collapse List of Standards

- Quick collapse / expand in Internal (performance) standards page added



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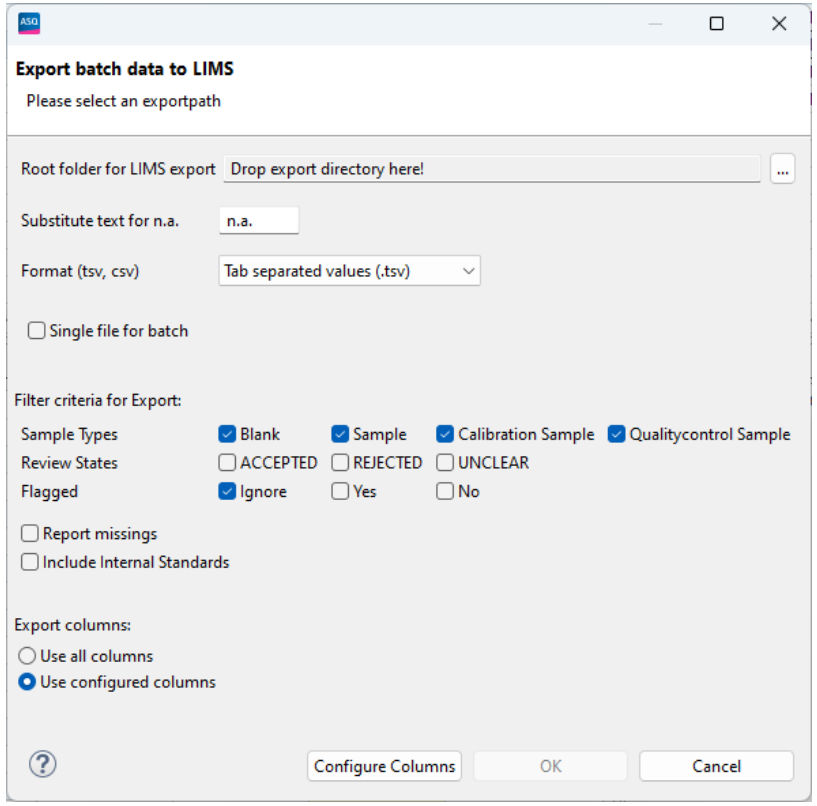
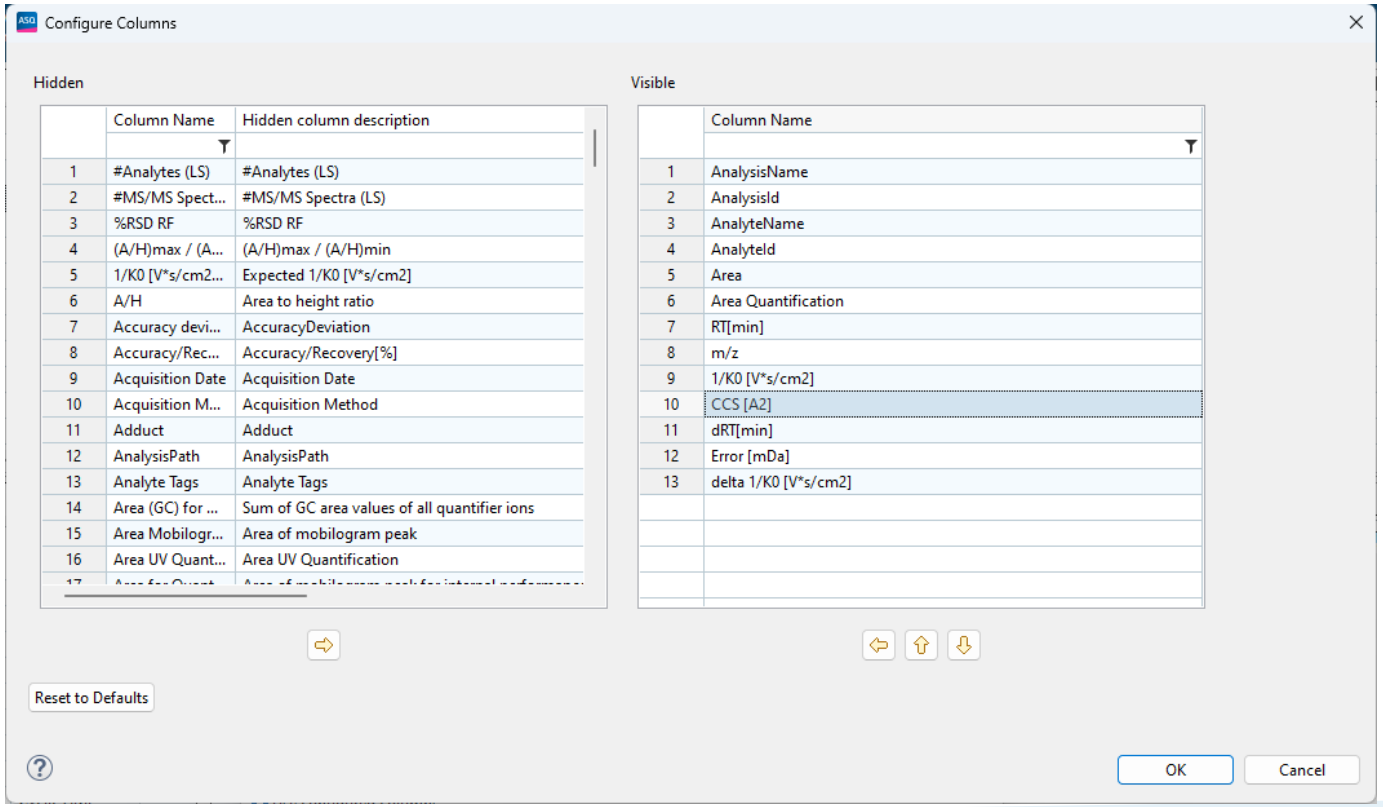
TASQ 2026B: Optionally Configure Columns to be Exported to LIMS File

- Currently only available for export to LIMS from client
- Future TASQ version will add LIMS column definition to TASQ processing method





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TASQ 2026B: Miscellaneous

- Method editor: Properly detect changes from „Single Peak“ to „Peak Group“ -> saving enabled
- Smart Formula view give a clear indication if NUPF processing service is not available
- Drag and Drop of concentrations.tsv to Batch Concentrations view
- Added PMI type [M-nH]n+ for ecTOF support. CI ionization creates [M-H]+ ions.
- Added new option to show only traces for found ions in Chromatogram/s, List Chromatograms, Mobilogram/s view

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TASQ 2026B: Miscelaneous

- Added a json export of determinations for BioCrates WebIdQ
- Create a json file for each data set in batch
- It contains determinations for all found and missing analytes
- For each determination the chromatograms, mobilograms, MS spectra are exported
- Additionally the parameter set for the analyte is exported as well

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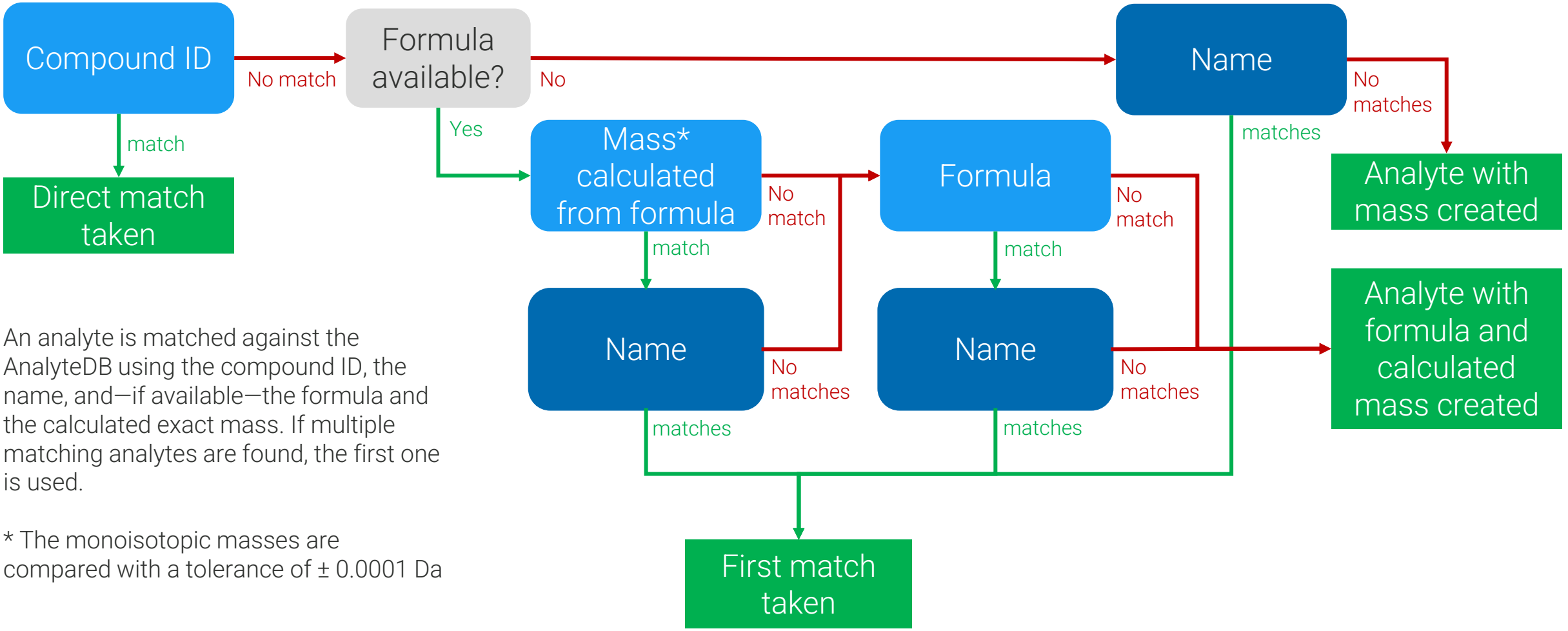
TASQ 2026B: How is an Analyte Identified During Import/ Create Method

(if during import, the option "Skip import of this analyte and keep existing one only" is chosen)



An analyte is matched against the AnalyteDB using the compound ID, the name, and—if available—the formula and the calculated exact mass. If multiple matching analytes are found, the first one is used.

* The monoisotopic masses are compared with a tolerance of ± 0.0001 Da

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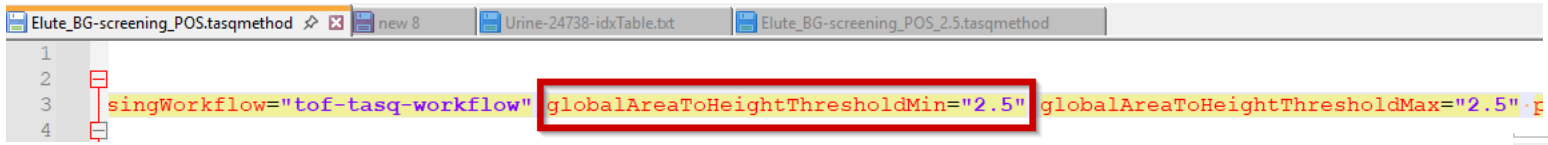
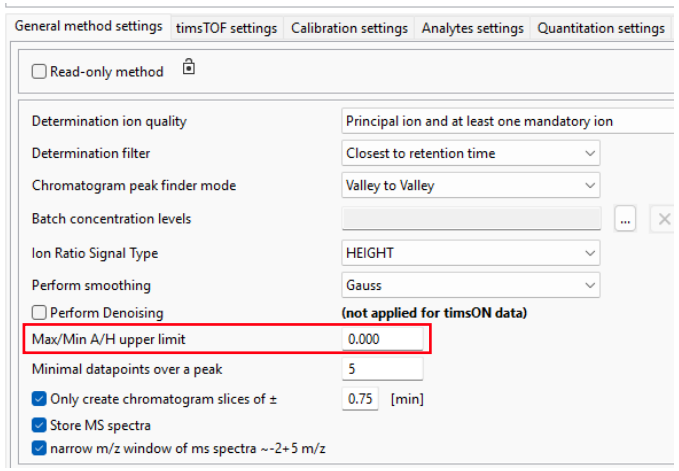
TASQ 2026B: Known Issues

- Customer reported missing determinations although ideal peaks are present.
  - Cause: A/H max filter was not properly implemented.
  - In TASQ 2026 and earlier the wrong property was used for A/H max filter.
  - Workaround: Export tasqMethod and change value for **globalAreaToHeightThresholdMin** to a higher value



  - This is fixed in TASQ 2026B.
  - If existing methods results in no findings after upgrade to TASQ 2026B
  - Check **Max/Min A/H upper** limit in **General method settings**



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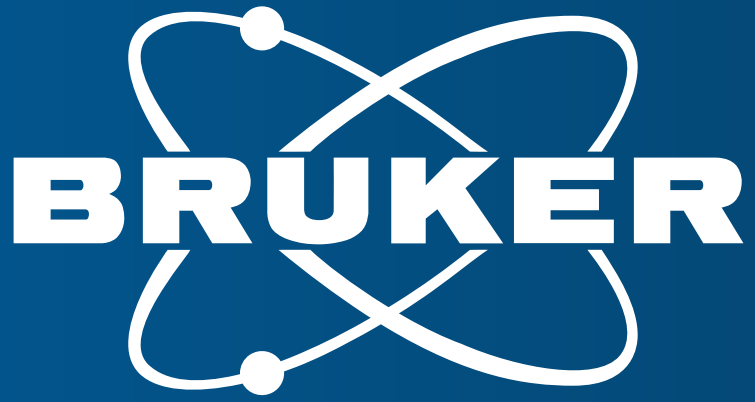

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