TASQ 2025B

What is new in TASQ 2025b

TASQ 2025b – Features

- Processing and quantification of UV-VIS data
  - UV-VIS data collected and stored by HyStar is supported (chromatography-data.sqlite)
  - MS data must also be acquired

TASQ 2025b – Features

- Processing
  - Load single wavelength UV-VIS chromatograms
  - Extract UV-VIS chromatograms from DAD spectra
  - Smooth traces
  - Perform peak detection and integration
    - Valley to valley option is currently not supported!
    - S/N filter currently not performed
  - Store peak data and group them to a determination
- Manual integration of UV-VIS chromatogram

TASQ 2025b – Features

- Quantification
  - Use UV-VIS area or height for regression calculation and calculation of quantities
  - Obey UV-VIS area or height of internal standard accordingly

TASQ 2025b: UV-VIS Processing Result Presentation – Result Tables

- Result table add Area/Height for Quantification (UV) column as summary on determination level
- Available columns for result tables

Area (UV) for Quantification	Sum of UV area values of all quantifier ions
Area for Quantification [IS] (UV)	Area of UV chromatogram peak for internal standard
Height (UV) for Quantification	Sum of UV height values of all quantifier ions
Height for Quantification [IS] (UV)	Height for Quantification [IS] (UV)
Rel. Area UV	Area UV relative to internal standard
Rel. Height UV	Height UV relative to internal standard
Rel. Quantity (UV Area)	Relative quant based on IS c= (S_A for Quantification UV / $S_{IS\,A}$ UV) * c_{IS}
Rel. Quantity (UV Height)	Relative quant based on IS c= (S_H for Quantification UV / $S_{IS\,H}$ UV) * c_{IS}

Analysis Results

	Analyte Name	Formula	MRSQC	Δm/z [mDa]	ΔRT [min]	mSigma	Quantity	Quantity expe...	Area (UV) for Quantification	Area for Quantification [IS] (UV)	Height (UV) for Quantification	Height for Quantification [IS] (UV)	Rel. Area UV	Rel. Height UV	Rel. Quantity (UV Area)	Rel. Quantity (UV Height)	A/H	Visited	Review State
1	Caffeine	$C_8H_{10}N_4O_2$		0.09	0.18	3.1	2510.7 ng/mL	2500.0 ng/mL	708		200						6.7	☑	ACCEPTED
2	Theobromine Mob1	$C_7H_8N_4O_2$		0.27	0.15	1.7	2772.1 ng/mL	2500.0 ng/mL	125	708	31	200	0.157	0.176	439.8 ng/mL	392.1 ng/mL	6.7	☑	ACCEPTED
3	Reserpine	$C_{33}H_{40}N_2O_9$		-0.28	0.40	9.2	264.8 ng/mL	250.0 ng/mL		708		200					8.3	☐	NONE
4	Alprazolam	$C_{17}H_{13}ClN_4$		-0.28	0.26	14.3	26.2 ng/mL	25.0 ng/mL									7.7	☐	NONE

TASQ 2025b: UV-VIS Processing Result Presentation – Detailed UV Results View

- New Detailed UV Results view available – displays results for the different UV-VIS traces specified for each analyte

Detailed UV Results

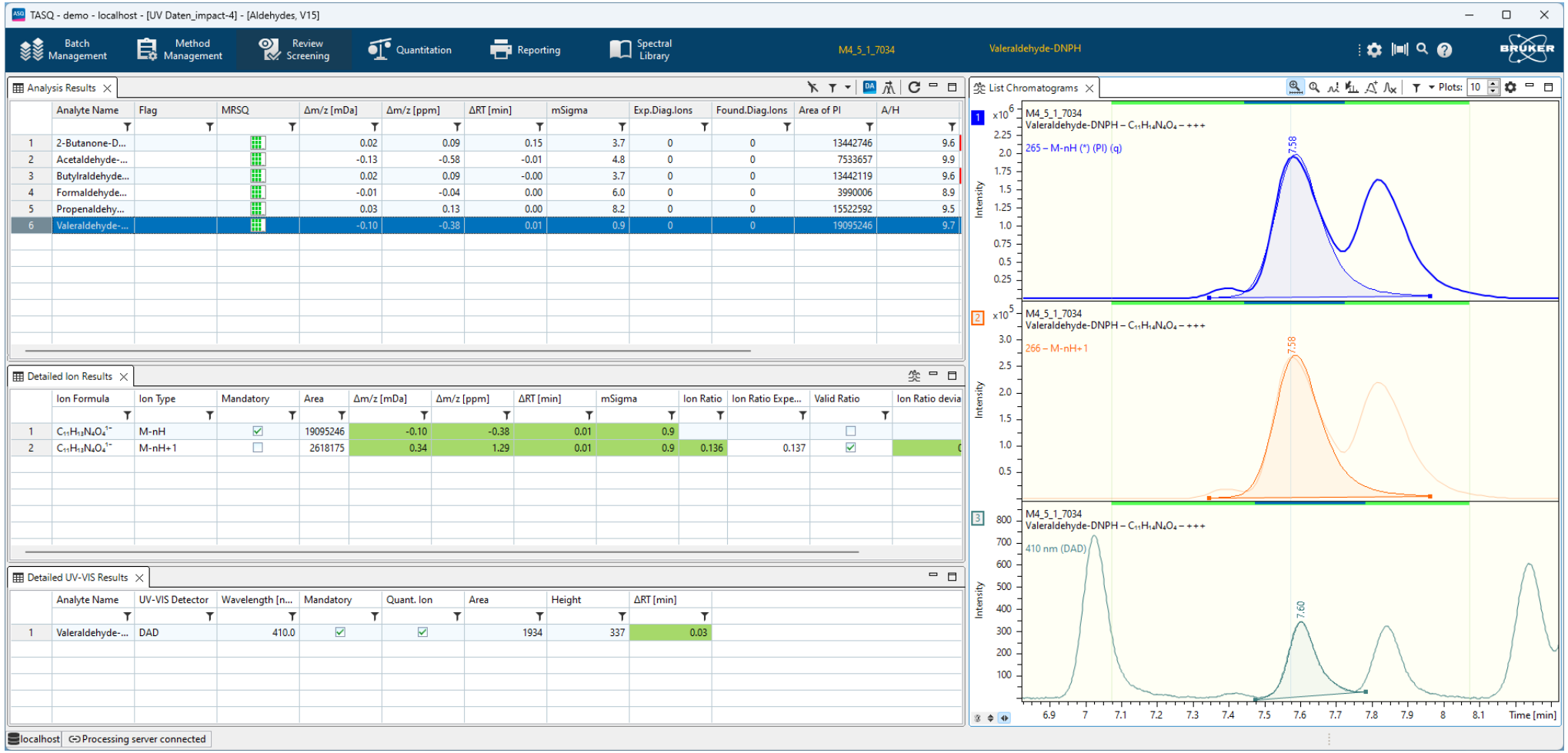
	Analyte Name	Wavelength [nm]	UV Detector	Status	RT expected [min]	RT [min]	RT Score	ΔRT [min]	FWHM [s]	Quant. Ion	Mandatory	Man.	Area	Height	Intensity	A/H	S/N	Noise	Found
1	Caffeine	280.0	DAD		4.27	4.45	++	0.18	3.30	☑	☐	☐	708	200	189	3.5	200	1	☑

TASQ 2025b: UV-VIS Processing Result Presentation

- New Detailed UV Results view available – displays results for the different UV-VIS traces specified for each analyte

A/H	Area to height ratio indicates whether this is a real chromatographic peak.
Analyte	Name of analyte
Area	Area of detected chromatographic peak for ion trace
FWHM [s]	Chromatographic peak width at half height in seconds
Found	Status information whether analyte has been identified or not
Height	Height of detected chromatographic peak for ion trace
Intensity	Intensity of detected chromatographic peak for ion trace
Man.	Flag whether peak has been integrated manually
Mandatory	Mandatory ion
Noise	Back calculated noise from S/N and S
Quant. Ion	Quantifier ion
RT Score	Retention time score
RT [min]	Observed retention time in minutes
RT expected [min]	Expected retention time in minutes
S/N	Signal-to-noise level of chromatographic peak for finding
Status	Status of measurement
UV Detector	Shows the used source of UV data (channel trace or DAD spectra)
Wavelength [nm]	Wavelength setting of UV chromatogram
ΔRT [min]	Absolute retention time deviation of finding relative to expected retention time

TASQ 2025b: Detailed UV-VIS Results View Available

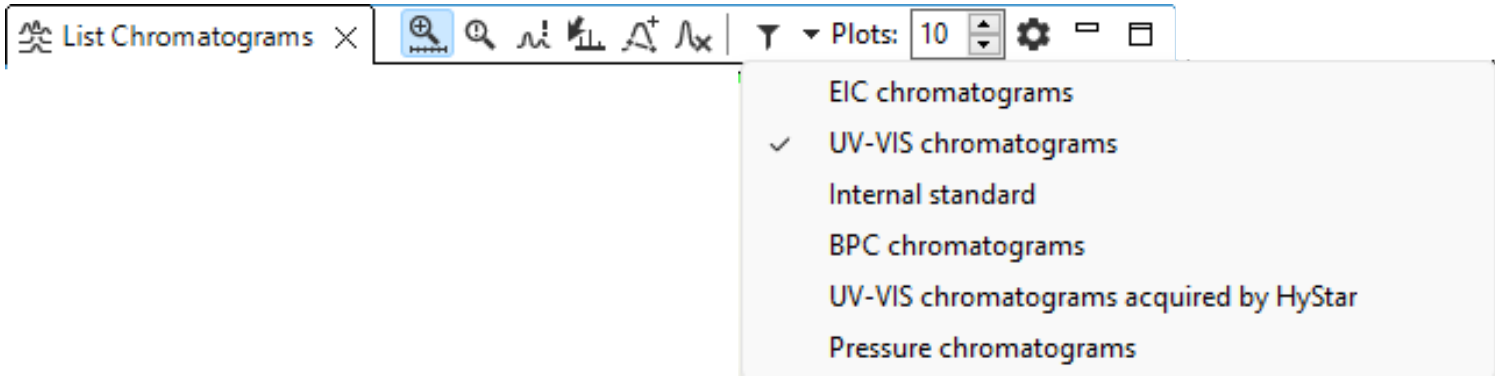


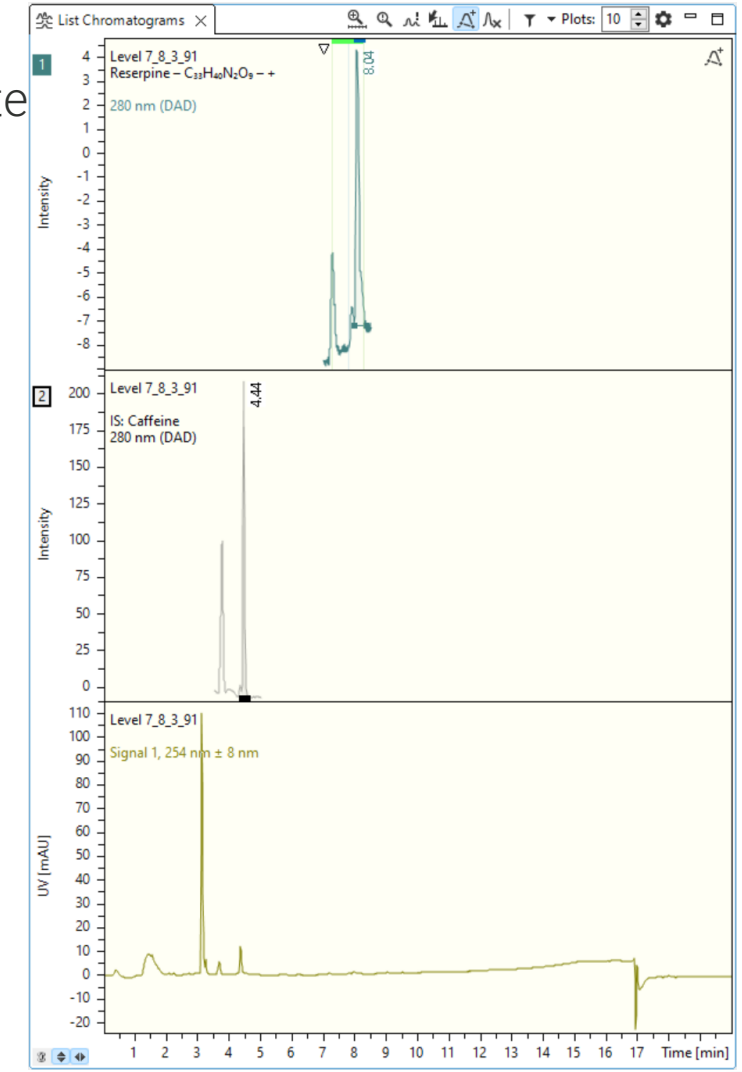
TASQ 2025b: UV-VIS Processing Result Presentation – List Chromatograms View

- List Chromatograms view displays the chromatographic traces and detected peaks for the specified UV-VIS traces
  - List Chromatograms view allows to integrate manually the peaks of the UV-VIS traces
- Show optionally UV-VIS traces of associated internal standard

TASQ 2025b: List Chromatogram View – UV-VIS chromatograms / Internal Standard

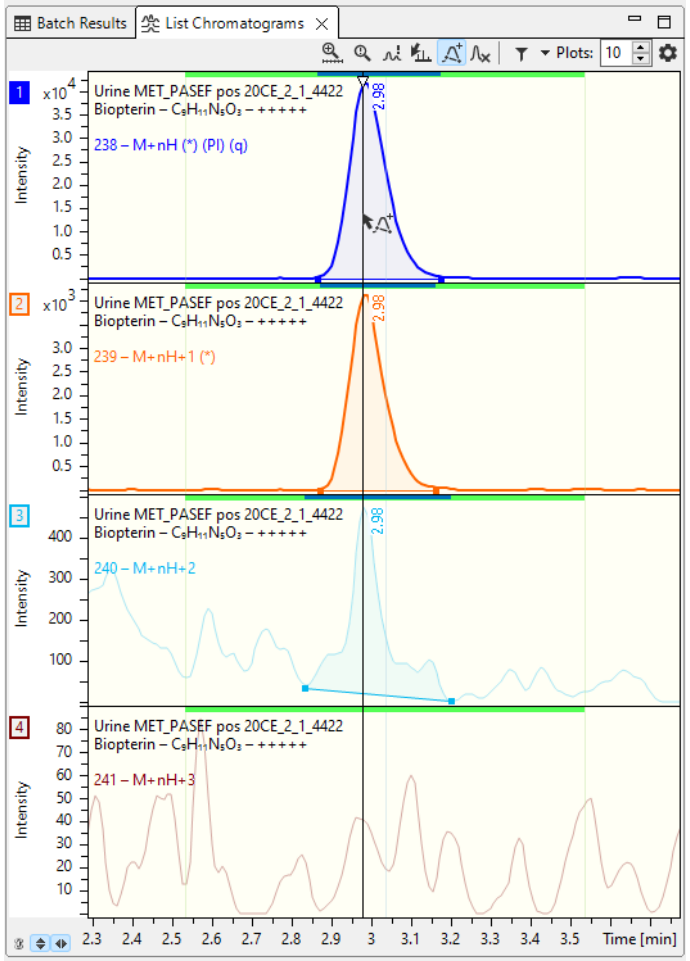
- Show all UV-VIS chromatograms available from chromatography-data.sqlite
- Show UV-VIS compound traces of selected analyte and optionally related internal standard
- Option to show / hide EIC chromatogram of selected determination

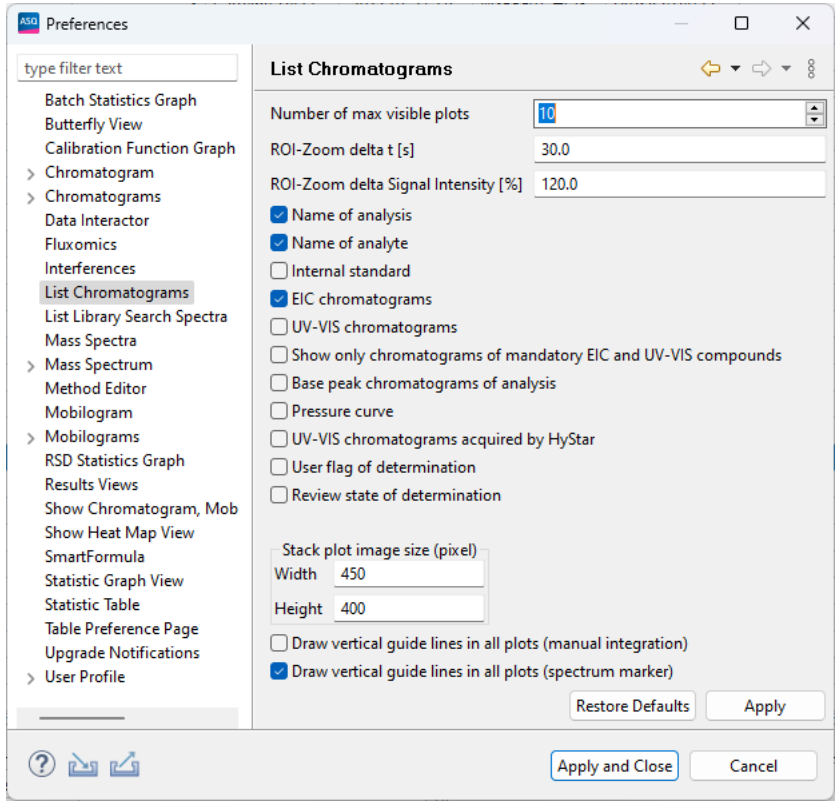




TASQ 2025b: List Chromatograms View – Vertical Guidelines

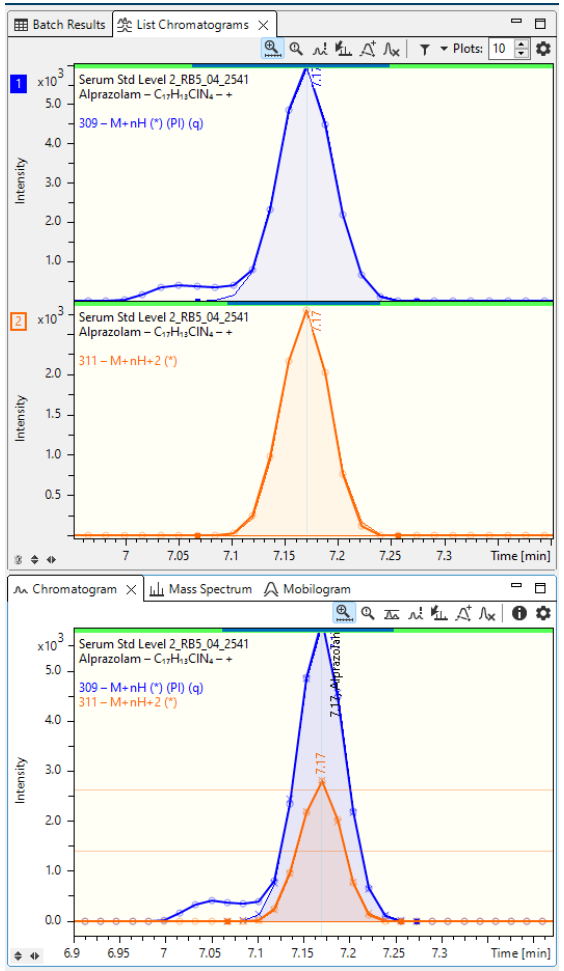
- Show vertical rulers in all views simultaneously to compare as a guide for comparison the various traces



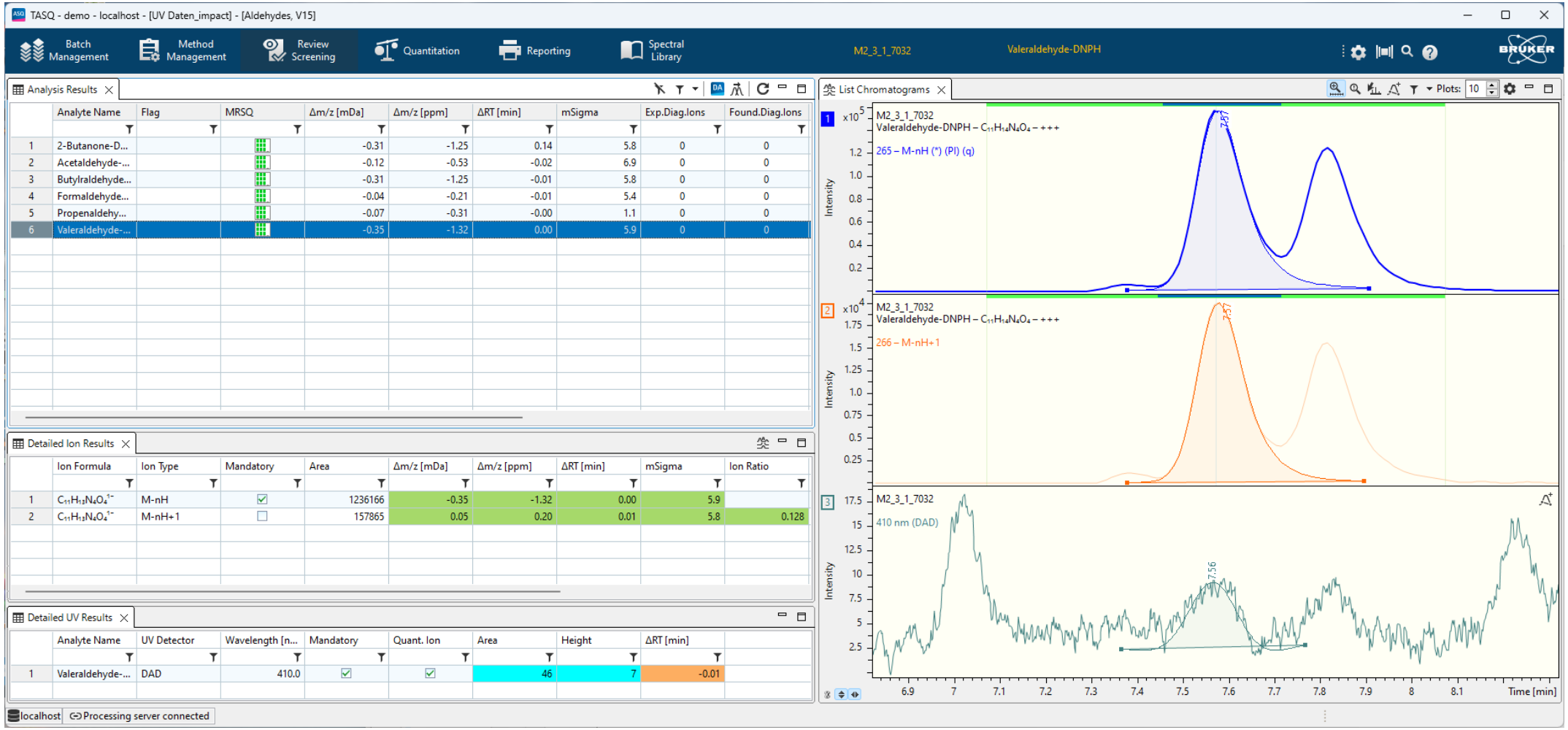


TASQ 2025b: List Chromatograms View: Show EMG Fitted Curves

- As in Chromatogram/s, Mobilogram/s view



TASQ 2025b: Detailed UV Results View Available



TASQ 2025b – UV-VIS Method Parameters

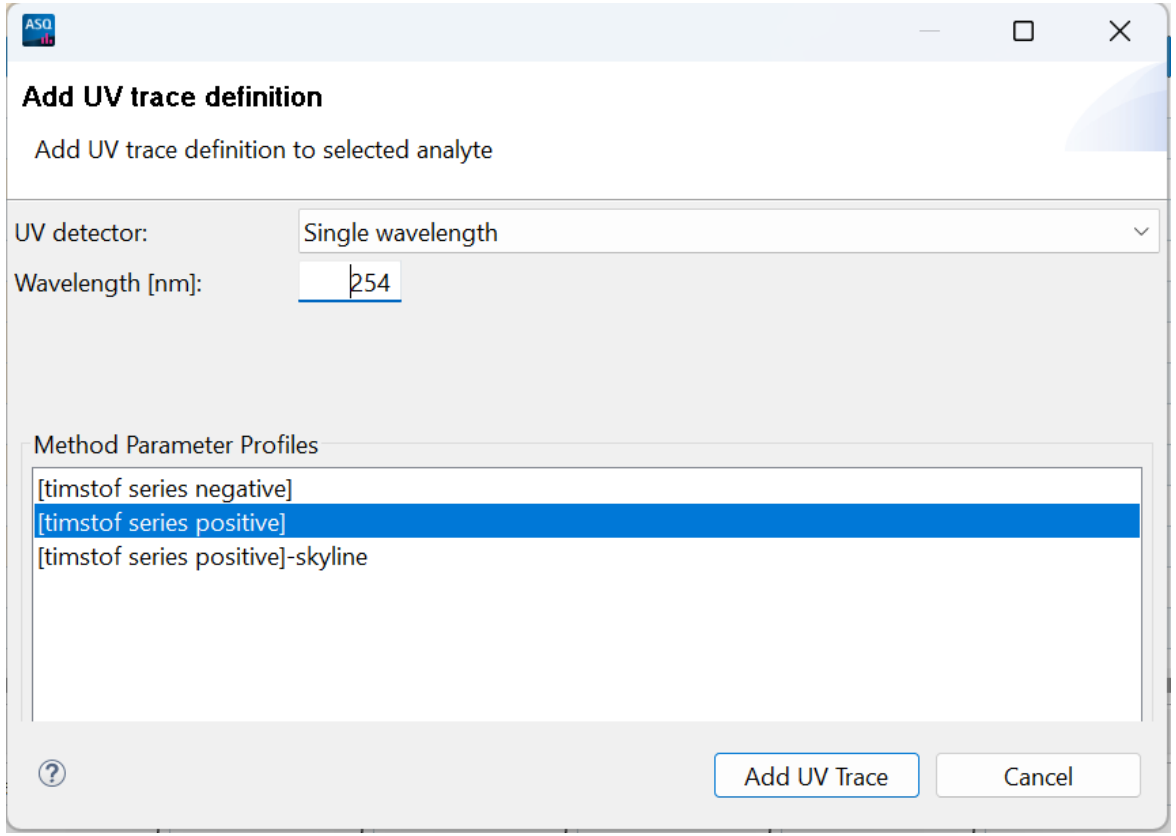
- In General Method Settings is a new group for detector configuration
  - If UV-VIS data is available specify the retention time offset of clock of the UV-VIS detector and the MS detector
- In the Analytes settings tab is a new sub tab beside of the Ions tab
  - Specify here the settings for loading or extracting UV-VIS chromatograms for single wavelength or DAD chromatograms

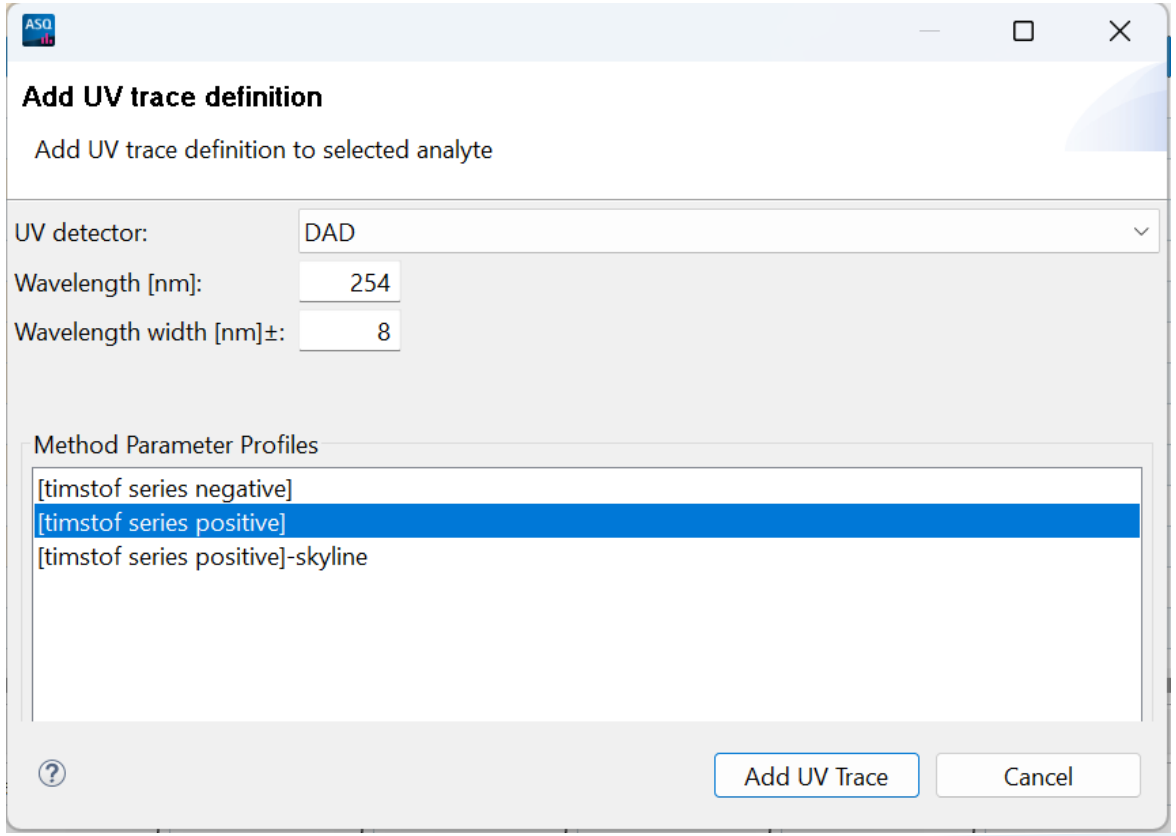
Ions | UV-VIS | Ion Ratios | Rules

	Analyte	UV-VIS Detector	Wavelength [n...	Wavelength wi...	Mandatory	Quant. UV-VIS ...	Area thr.	Height thr.	Sens. [%]	Min peak valle...	Smoothing wi...
1	Caffeine	DAD	280	10	☐	☑	0	0	90	4.0	0.10
2	Reserpine	DAD	280	10	☐	☑	0	0	90	4.0	0.10
3	Theobromine ...	DAD	280	10	☐	☑	0	0	90	4.0	0.10
4	Theobromine ...	DAD	254	10	☐	☑	0	0	90	4.0	0.10

TASQ 2025b – UV-VIS Method Parameters: Add a UV-VIS Trace

- UV-VIS chromatograms can be acquired as single wavelength chromatograms stored by HyStar or
- Extracted UV-VIS chromatograms calculated from DAD UV-VIS spectra



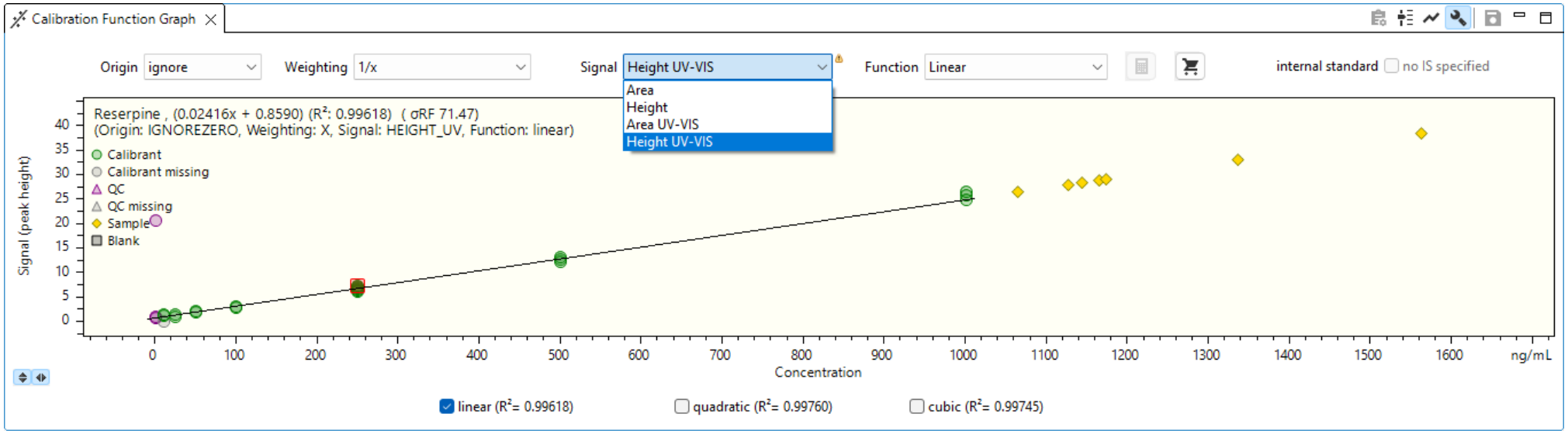


TASQ 2025b – UV-VIS Quantitation Parameters

- For quantification specify Area or Height UV to use the UV-VIS derived signal values

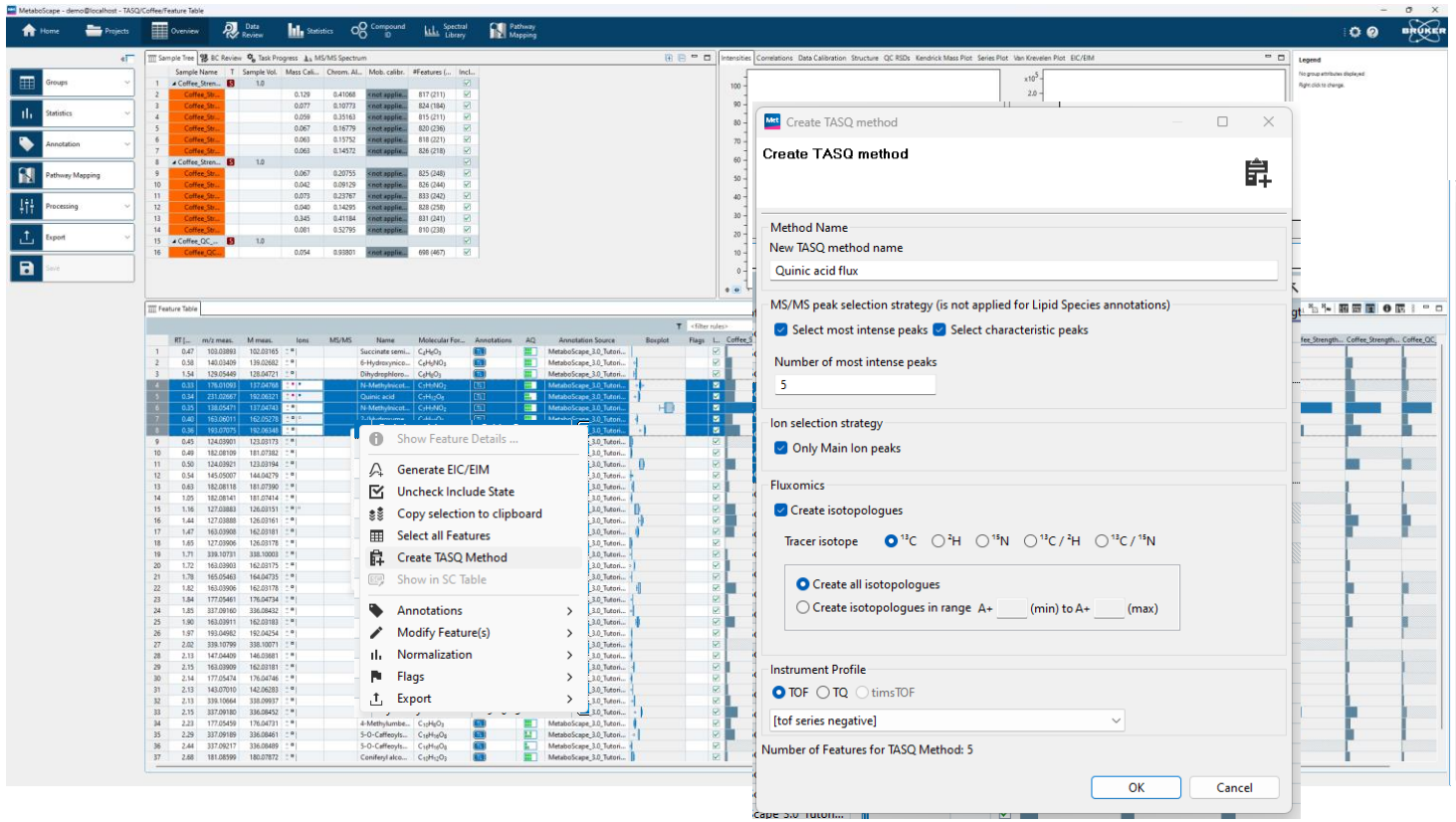
General method settings | Calibration settings | Analytes settings | Quantitation settings | Library search settings | General library search settings | Internal standards | Number formats | Colors definition | Workflow settings

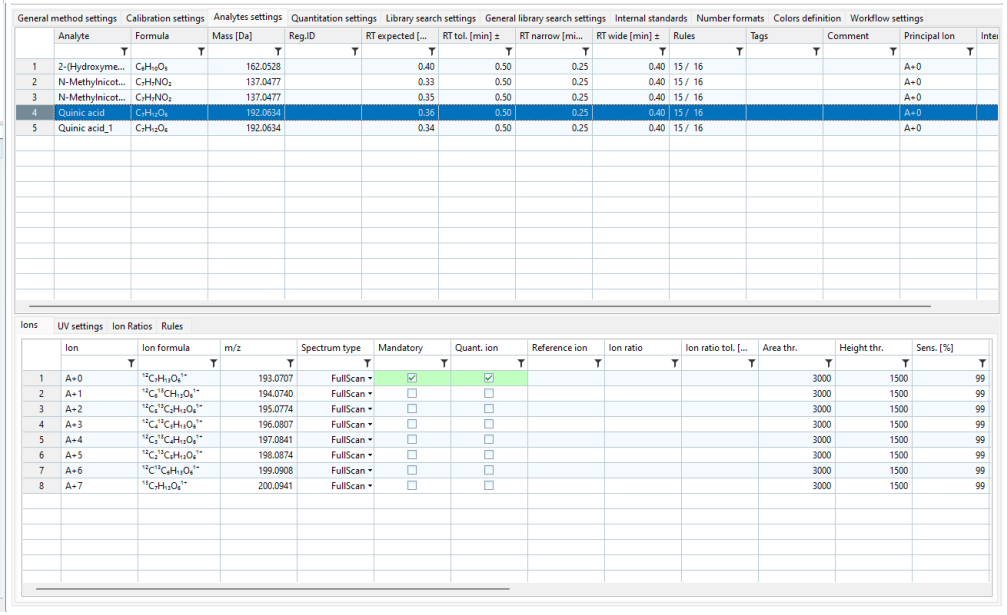
	Analyte	Function type	Weighting	Origin	Signal	Principal Ion	Quantitation ...	Correction fact...	Referenced an...	Tags	Legacy Calibra...	Interferences	Batch origin
1	Caffeine	Linear	None	Force	Area	M+nH	IN_BATCH	1.000	Caffeine				
2	Reserpine	Linear	1/x	Ignore	Area	M+nH	IN_BATCH	1.000	Reserpine				
3	Theobromine ...	Linear	1/x	Ignore	Height	M+nH	IN_BATCH	1.000	Theobromine ...				
4	Theobromine ...	Linear	1/x	Ignore	Area UV-VIS	M+nH	IN_BATCH	1.000	Theobromine ...				
					Height UV-VIS								



TASQ 2025b – Method Creation in MetaboScape

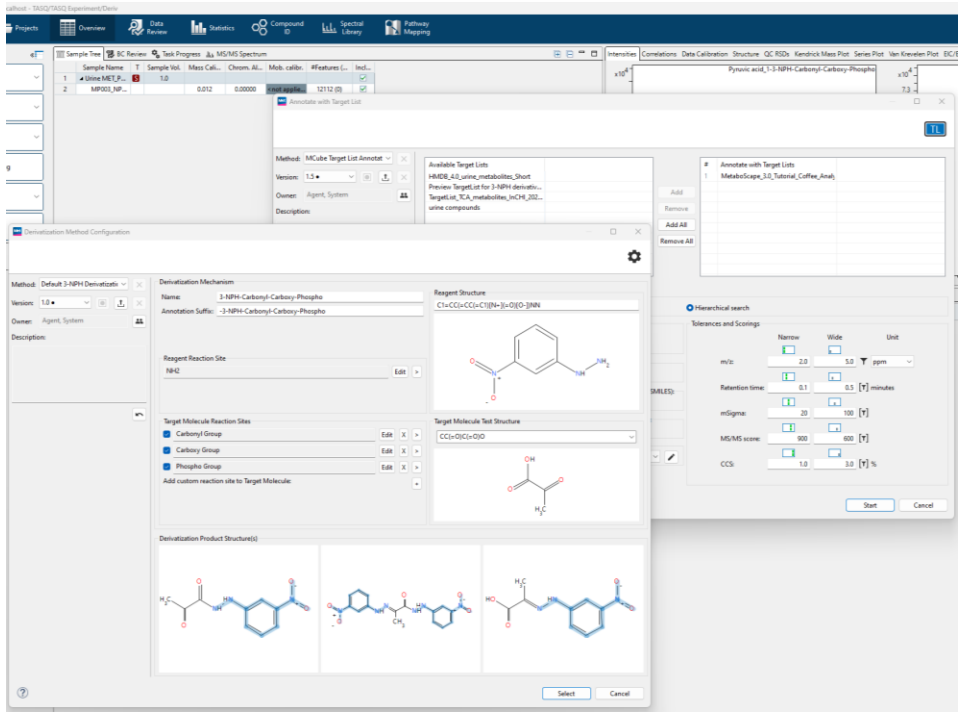
- Extension for fluxomics/derivatisation – Create TASQ method from MetaboScape
  - Support for fluxomics w/ or w/o derivatisation

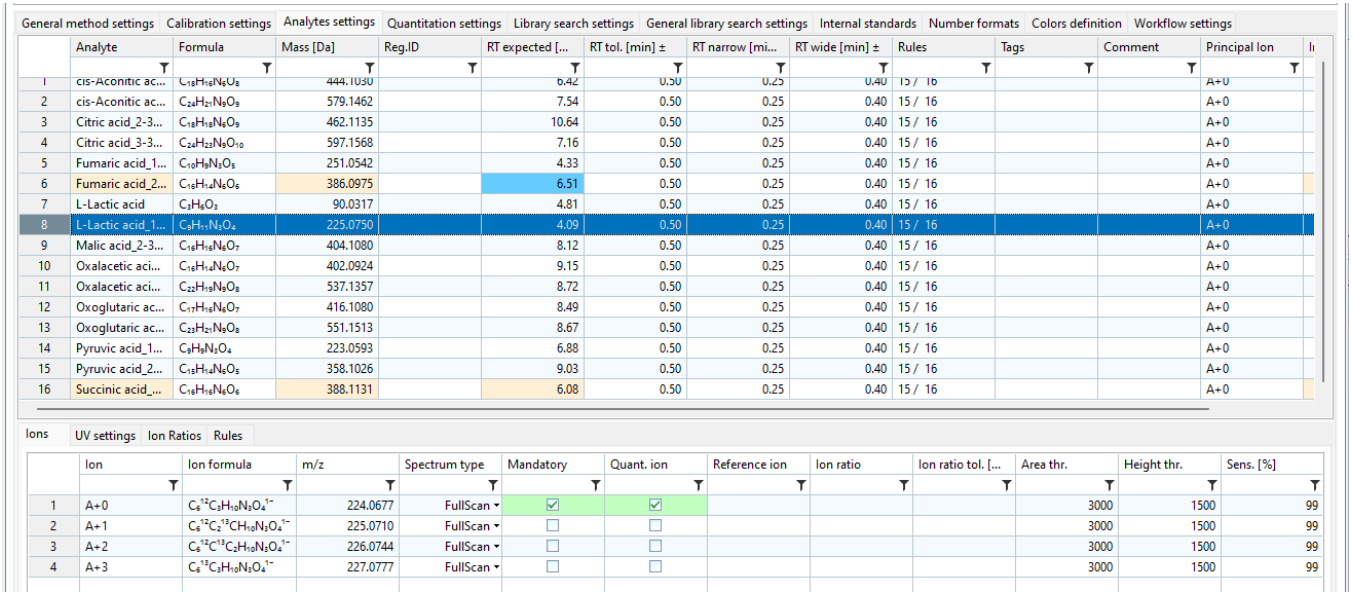




TASQ 2025b – Method Creation in MetaboScape

- Extension for fluxomics/derivatisation – Create TASQ method from MetaboScape
  - Support for fluxomics w/ or w/o derivatization – the moiety introduced by derivatization will not be considered for generation of isotopologous





General method settings | Calibration settings | Analytes settings | Quantitation settings | Library search settings | General library search settings | Internal standards | Number formats | Colors definition | Workflow settings

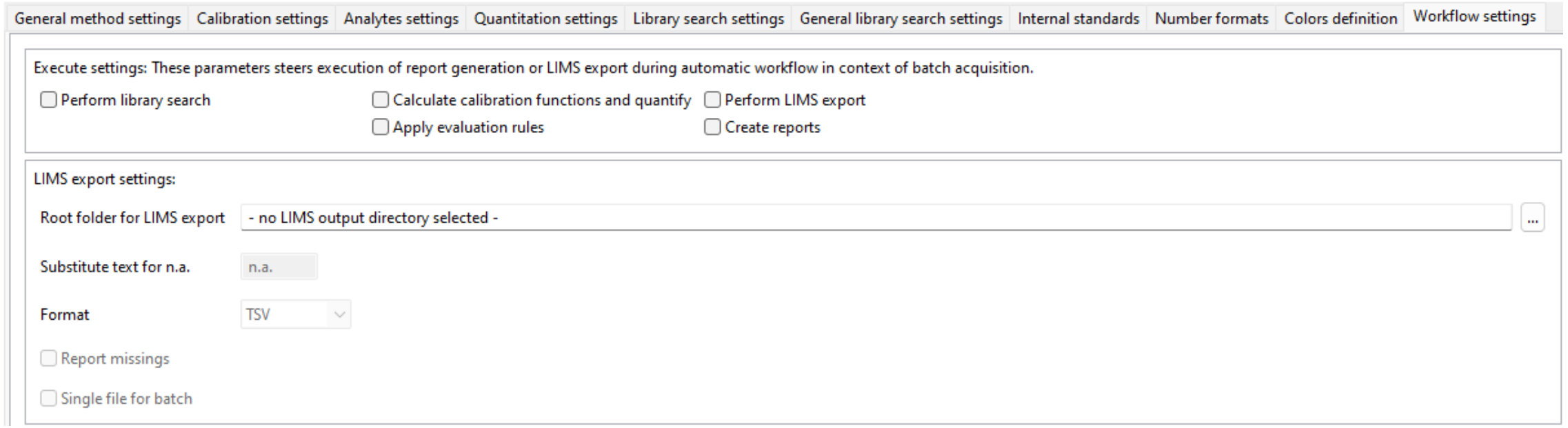
	Analyte	Formula	Mass [Da]	Reg.ID	RT expected [...	RT tol. [min] ±	RT narrow [mi...	RT wide [min] ±	Rules	Tags	Comment	Principal Ion
1	cis-Aconitic ac...	$C_{18}H_{16}N_6O_6$	444.1030		6.42	0.50	0.25	0.40	15 / 16			A+0
2	cis-Aconitic ac...	$C_{24}H_{21}N_9O_9$	579.1462		7.54	0.50	0.25	0.40	15 / 16			A+0
3	Citric acid_2-3...	$C_{18}H_{18}N_6O_9$	462.1135		10.64	0.50	0.25	0.40	15 / 16			A+0
4	Citric acid_3-3...	$C_{24}H_{23}N_9O_{10}$	597.1568		7.16	0.50	0.25	0.40	15 / 16			A+0
5	Fumaric acid_1...	$C_{10}H_8N_2O_6$	251.0542		4.33	0.50	0.25	0.40	15 / 16			A+0
6	Fumaric acid_2...	$C_{16}H_{14}N_6O_6$	386.0975		6.51	0.50	0.25	0.40	15 / 16			A+0
7	L-Lactic acid	$C_3H_6O_3$	90.0317		4.81	0.50	0.25	0.40	15 / 16			A+0
8	L-Lactic acid_1...	$C_9H_{11}N_3O_4$	225.0750		4.09	0.50	0.25	0.40	15 / 16			A+0
9	Malic acid_2-3...	$C_{16}H_{16}N_6O_7$	404.1080		8.12	0.50	0.25	0.40	15 / 16			A+0
10	Oxalacetic aci...	$C_{16}H_{14}N_6O_7$	402.0924		9.15	0.50	0.25	0.40	15 / 16			A+0
11	Oxalacetic aci...	$C_{22}H_{19}N_9O_8$	537.1357		8.72	0.50	0.25	0.40	15 / 16			A+0
12	Oxoglutaric ac...	$C_{17}H_{16}N_6O_7$	416.1080		8.49	0.50	0.25	0.40	15 / 16			A+0
13	Oxoglutaric ac...	$C_{23}H_{21}N_9O_8$	551.1513		8.67	0.50	0.25	0.40	15 / 16			A+0
14	Pyruvic acid_1...	$C_9H_9N_3O_4$	223.0593		6.88	0.50	0.25	0.40	15 / 16			A+0
15	Pyruvic acid_2...	$C_{15}H_{14}N_6O_9$	358.1026		9.03	0.50	0.25	0.40	15 / 16			A+0
16	Succinic acid_...	$C_{16}H_{18}N_6O_8$	388.1131		6.08	0.50	0.25	0.40	15 / 16			A+0

Ions | UV settings | Ion Ratios | Rules

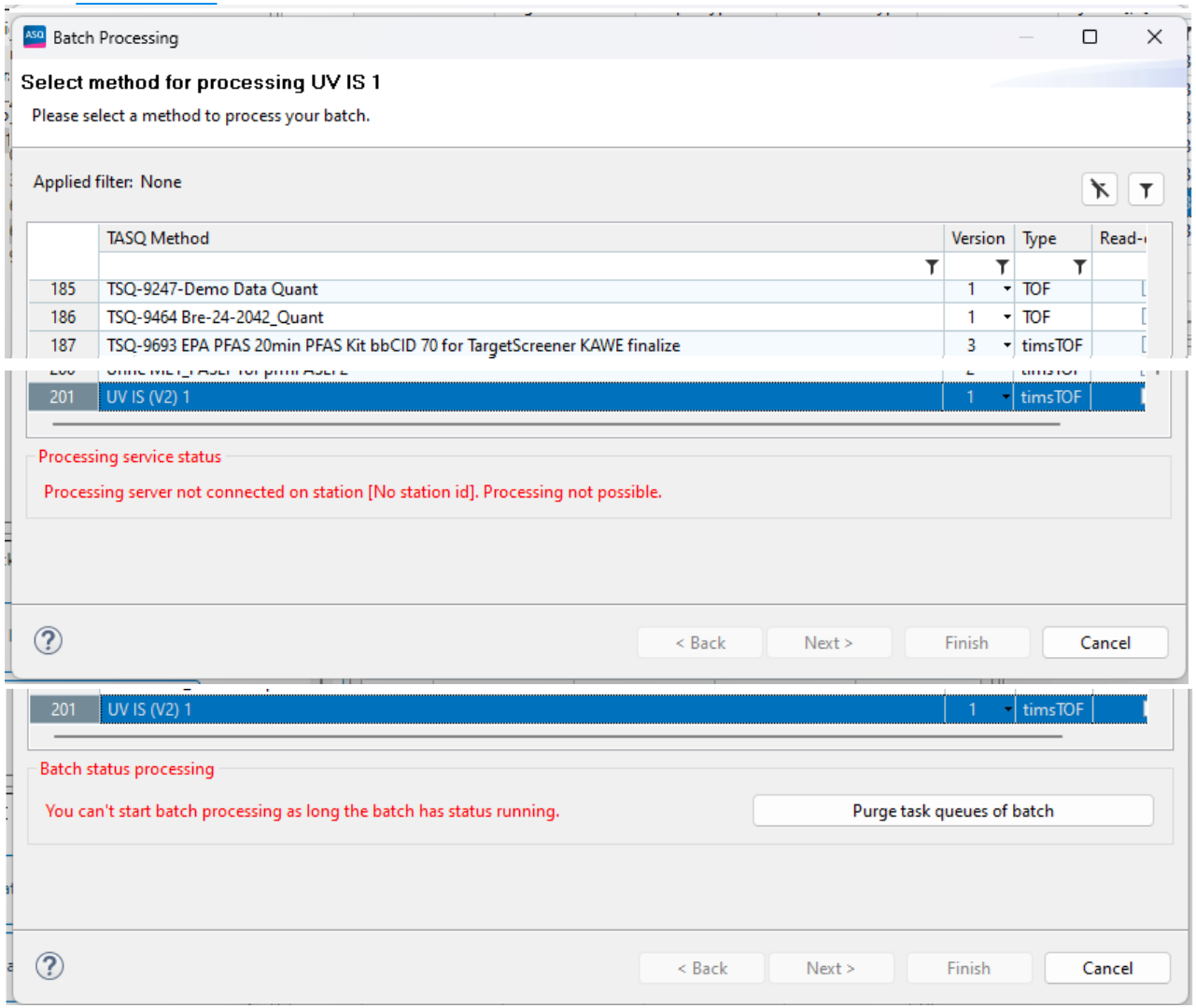
	Ion	Ion formula	m/z	Spectrum type	Mandatory	Quant. ion	Reference ion	Ion ratio	Ion ratio tol. [...	Area thr.	Height thr.	Sens. [%]
1	A+0	$C_6{}^{12}C_3H_{10}N_2O_4{}^{1-}$	224.0677	FullScan	☑	☑				3000	1500	99
2	A+1	$C_6{}^{12}C_2{}^{13}CH_{10}N_2O_4{}^{1-}$	225.0710	FullScan	☐	☐				3000	1500	99
3	A+2	$C_6{}^{12}C{}^{13}C_2H_{10}N_2O_4{}^{1-}$	226.0744	FullScan	☐	☐				3000	1500	99
4	A+3	$C_6{}^{13}C_3H_{10}N_2O_4{}^{1-}$	227.0777	FullScan	☐	☐				3000	1500	99

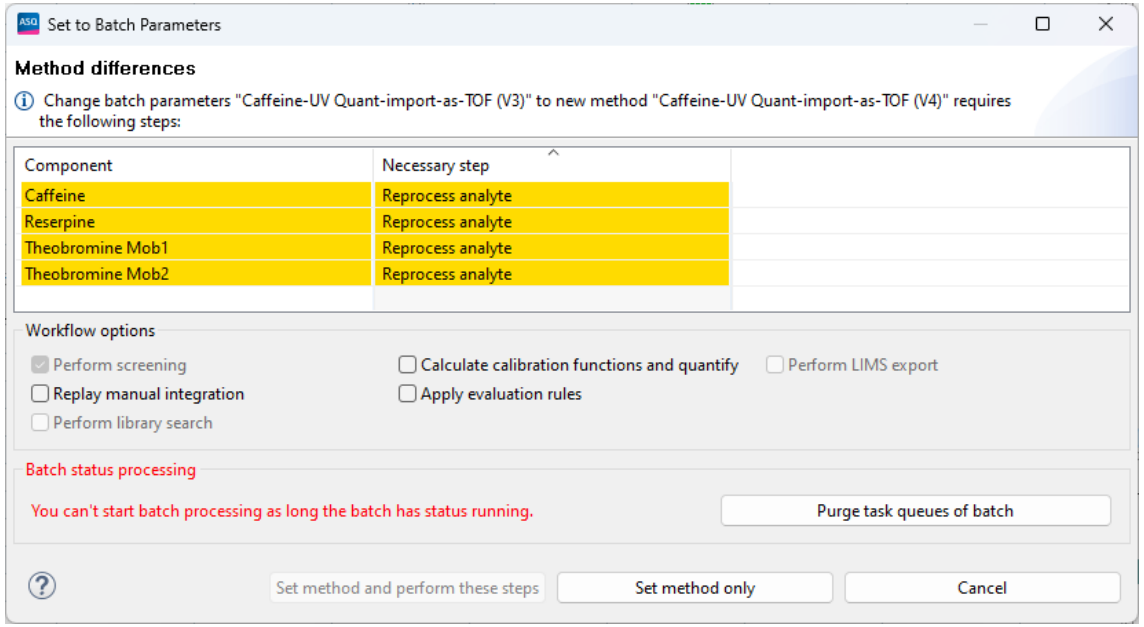
TASQ 2025b – User Workflow – Process Batch

- Add Perform Library Search and Apply Evaluation Rules as seperate workflow steps to Workflow Settings tab



TASQ 2025b: Checks Whether a Batch can be Processed



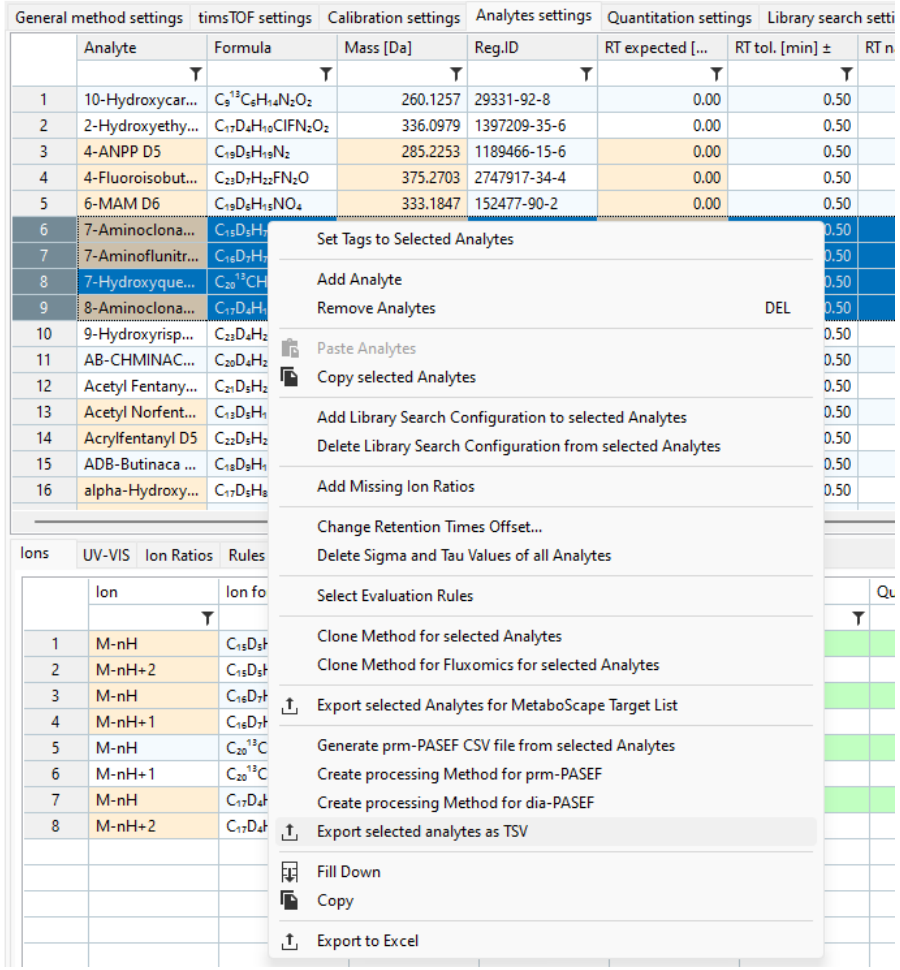


TASQ 2025b: Improvements

- DART – make use of area / intensity threshold for detection of analytes
- TASQ method: disable Peak Fit option if DART processing is selected

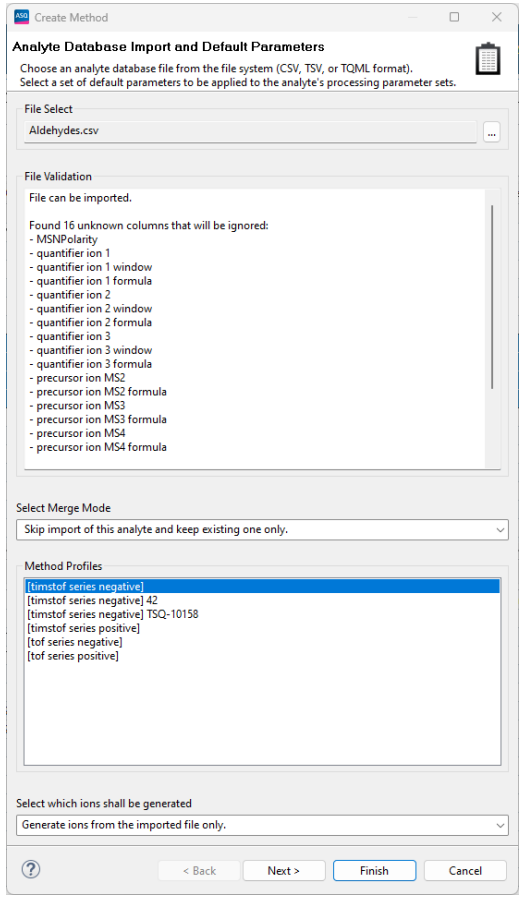
TASQ 2025b: Export Parameter Settings of Selected Analytes

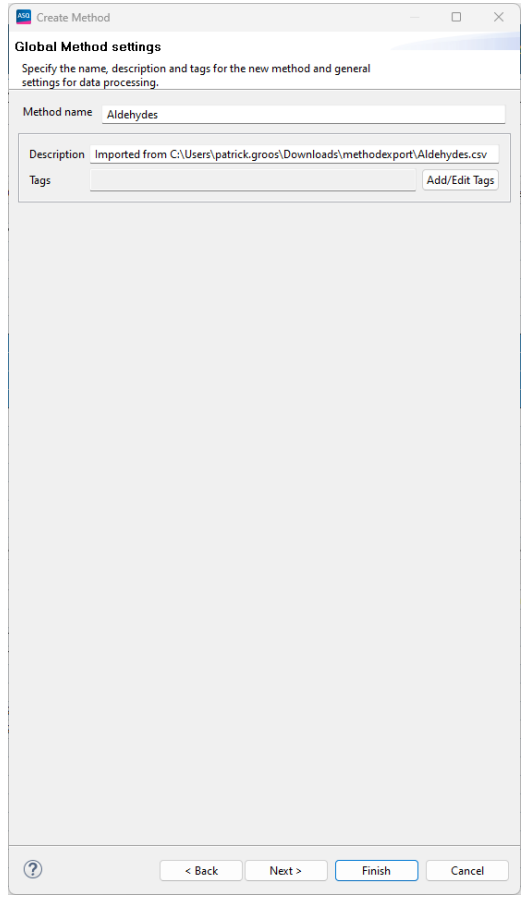
- Export all processing parameter of selected analytes in a TASQ method as a tab seperated text file
- This parameter sets can be modified in any text editor or Excel

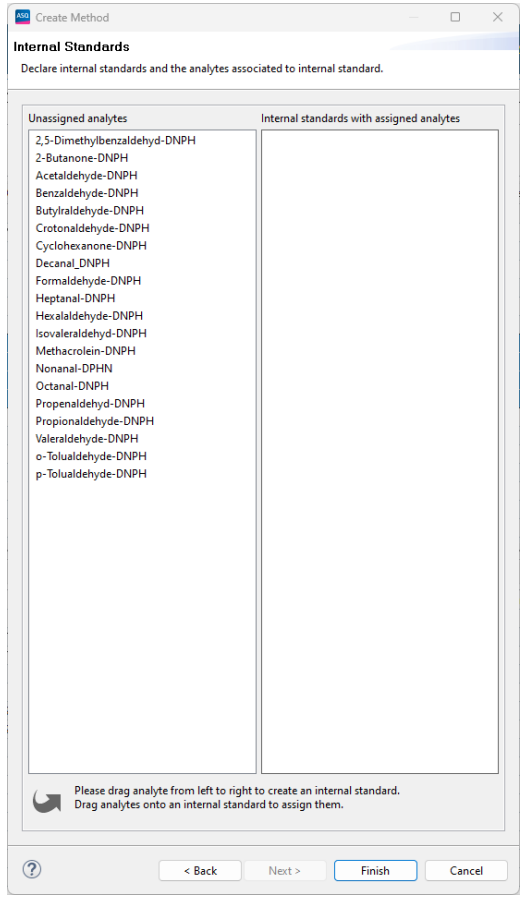


TASQ 2025b: Import new TSV File for Creating a TASQ Method

- Import modified parameter sets as a new method

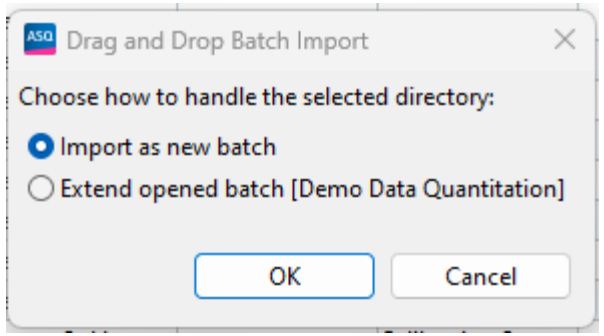






TASQ 2025b: Drag & Drop – Acquired Data, TASQ Method, BRKRAR

- Import .brkrar file on drag & drop from file explorer to Batch Summary view
  - Import batch – drag & drop folder containing .d data sets
  - Extend batch –drag & drop .d folders
  - Import .tasqMethod
  - Import .brkrar (new)
- Create TASQ processing method by drag & drop of .csv, .tsv, or .tqml analyte specifications (new)

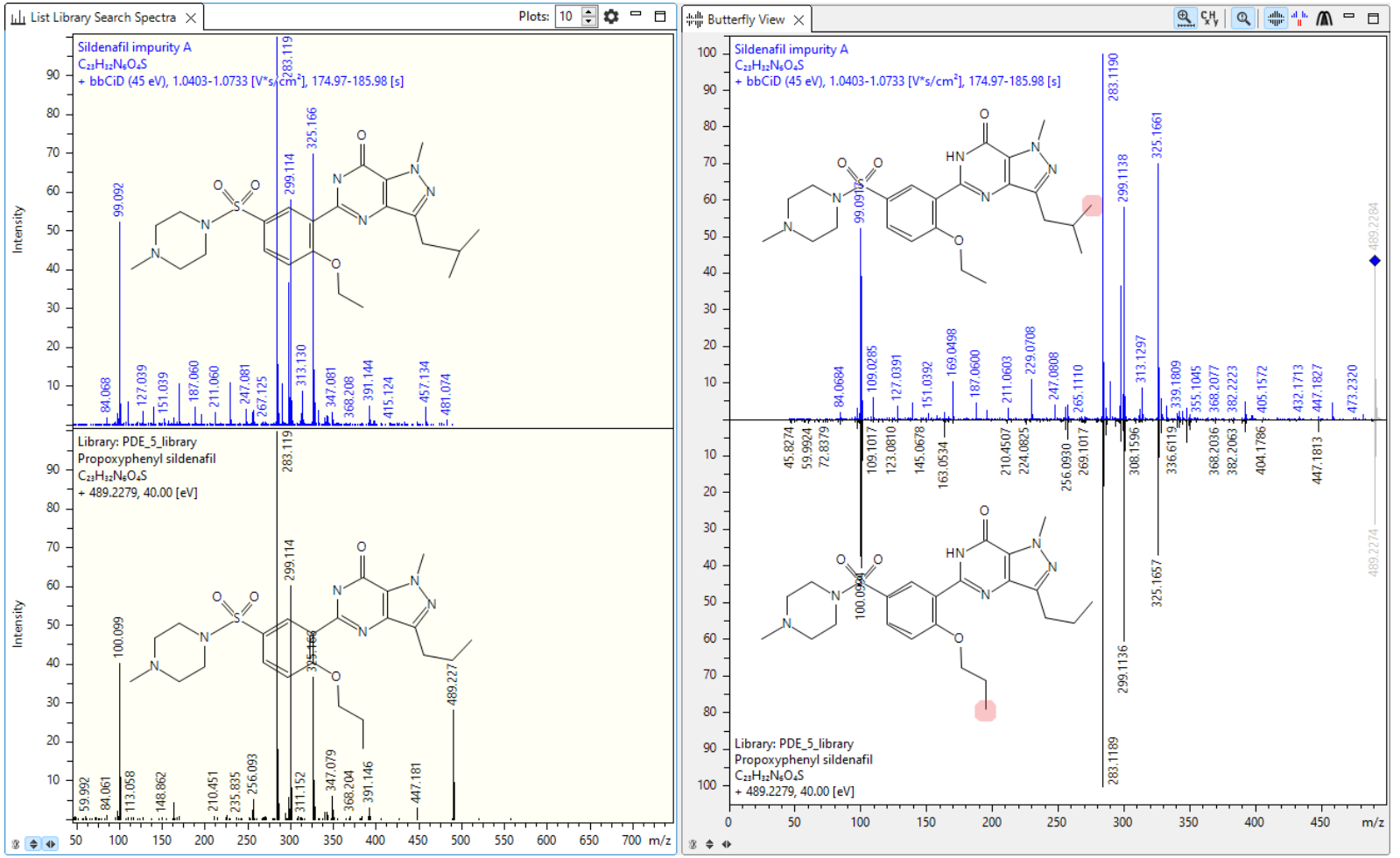


TASQ 2025b: Library Search

- Show structure of TASQ method compound or library search compound in List Library Search Spectra view
- Optionally highligth common or different structure moieties in chemical structure in Butterfly view
- Added Smart Formula pointer to Butterfly view
  - Click on a peak in acquired spectrum or library spectrum to generate elemental compositions and optionally add the identified fragment peak to TASQ method
- New method parameter on Genearl library search settings tab – Fragment mass tolerance [mDa] for matching MS/MS peaks in library search spectrum
- Extend library search result info with time stamp when library search was performed
- When cloning a TASQ method add name and version of source to description

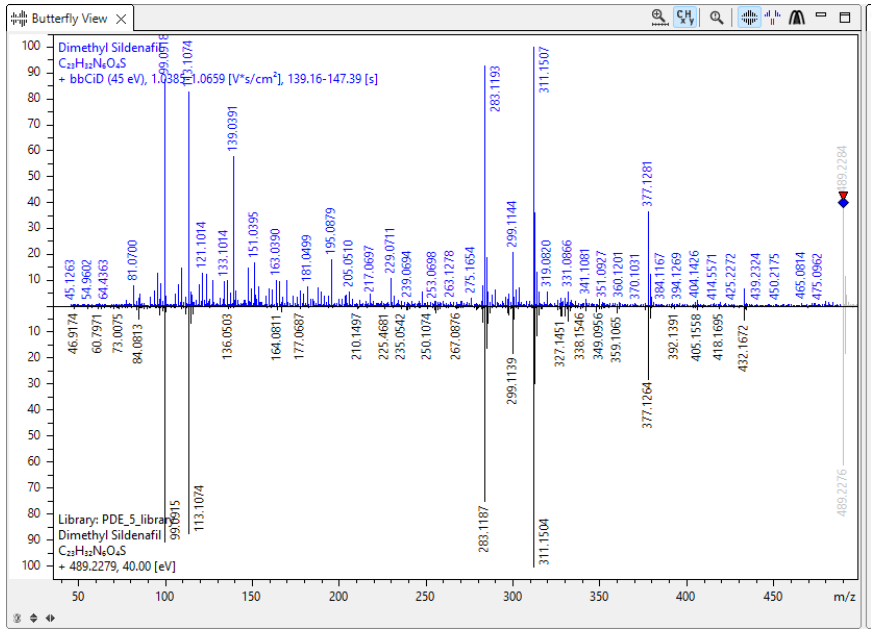
TASQ 2025b: news

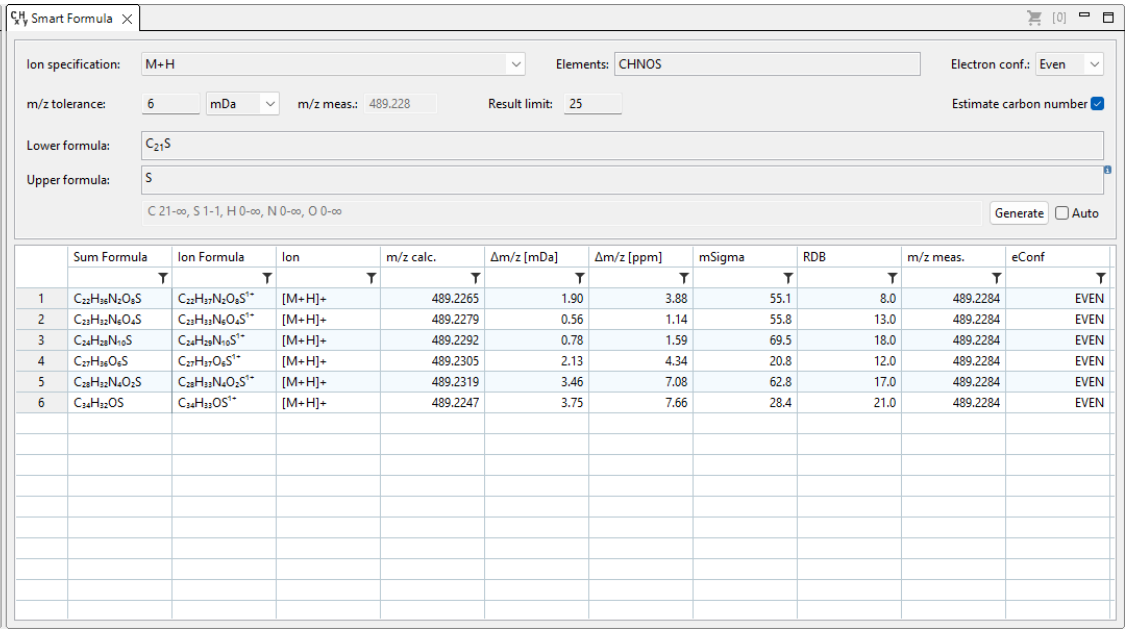
- Library Search Spectra list view
  - Show structure of compound
- Butterfly view
  - Show structure of compounds
    - TASQ method compound
    - Library spectrum compound
  - Highlight common substructure optionally
  - Highlight non-common substructure optionally



TASQ 2025b: SmartFormula from Butterfly View

- Peform SmartFormula from Butterfly view
- Click on a peak in measured spectrum or library spectrum and review results
- Add ions from SmartFormula view to TASQ method





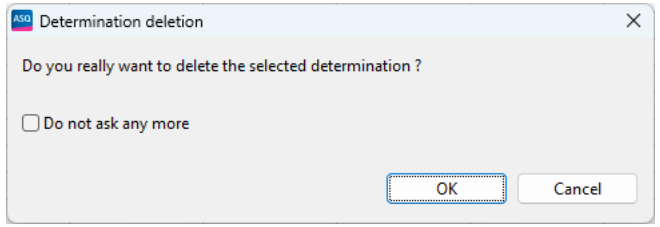
	Sum Formula	Ion Formula	Ion	m/z calc.	Δm/z [mDa]	Δm/z [ppm]	mSigma	RDB	m/z meas.	eConf
1	$C_{22}H_{36}N_2O_8S$	$C_{22}H_{37}N_2O_8S^{1+}$	[M+H]+	489.2265	1.90	3.88	55.1	8.0	489.2284	EVEN
2	$C_{23}H_{32}N_6O_4S$	$C_{23}H_{33}N_6O_4S^{1+}$	[M+H]+	489.2279	0.56	1.14	55.8	13.0	489.2284	EVEN
3	$C_{24}H_{28}N_{10}S$	$C_{24}H_{29}N_{10}S^{1+}$	[M+H]+	489.2292	0.78	1.59	69.5	18.0	489.2284	EVEN
4	$C_{27}H_{36}O_6S$	$C_{27}H_{37}O_6S^{1+}$	[M+H]+	489.2305	2.13	4.34	20.8	12.0	489.2284	EVEN
5	$C_{28}H_{32}N_4O_2S$	$C_{28}H_{33}N_4O_2S^{1+}$	[M+H]+	489.2319	3.46	7.08	62.8	17.0	489.2284	EVEN
6	$C_{34}H_{32}OS$	$C_{34}H_{33}OS^{1+}$	[M+H]+	489.2247	3.75	7.66	28.4	21.0	489.2284	EVEN

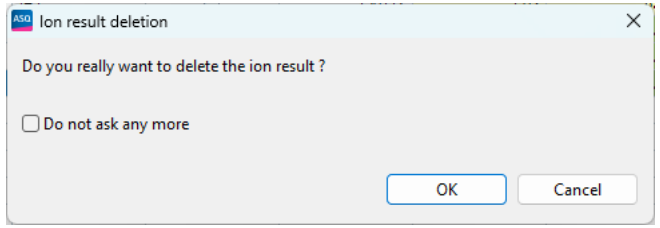
TASQ 2025b: Miscellaneous

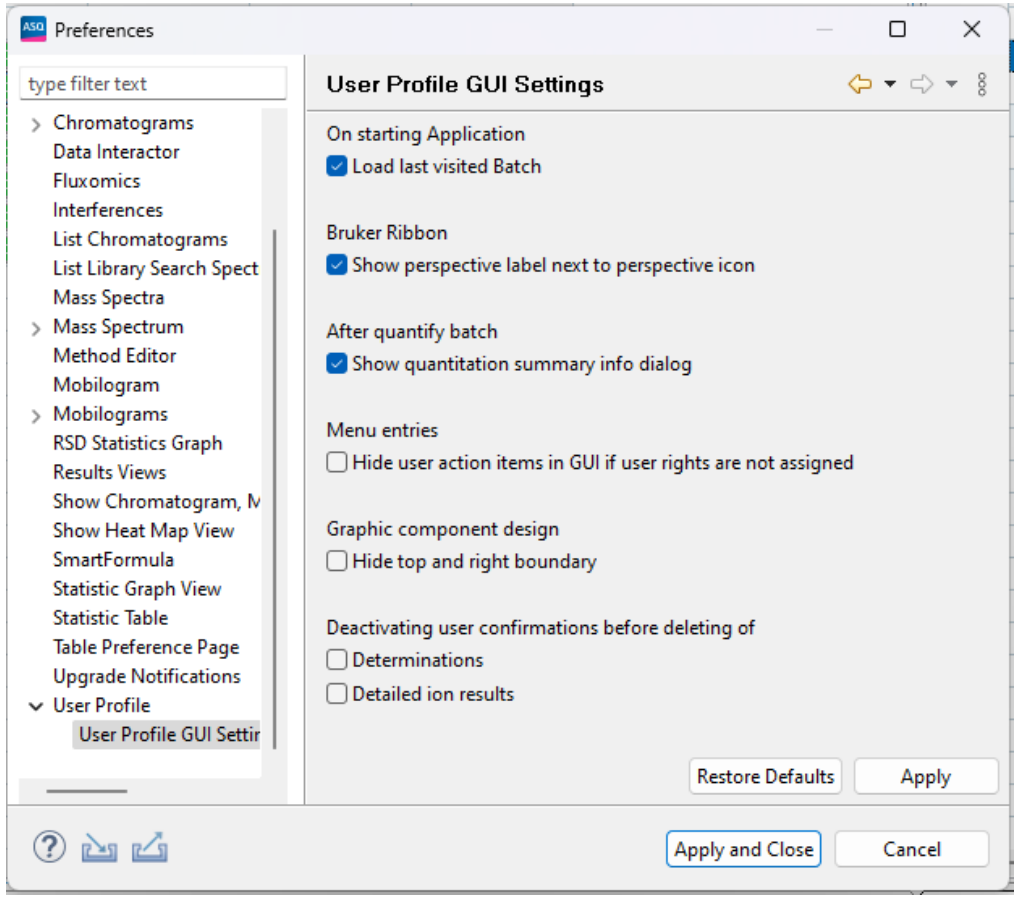
- Task Progress view can show tasks running on other stations optionally
- Ongoing improvements on handling context menu
- Ongoing work on import TASQ method from tsv file
- When cloning a TASQ method add name and version of source to description

TASQ 2025b: Miscellaneous

- Make behavior of Delete Ion Results and Delete Determination similar:
  - Show pop up dialog „really delete?“ in both cases
  - Add option to hide dialog next time
  - Can be switched on/off in Preferences as well

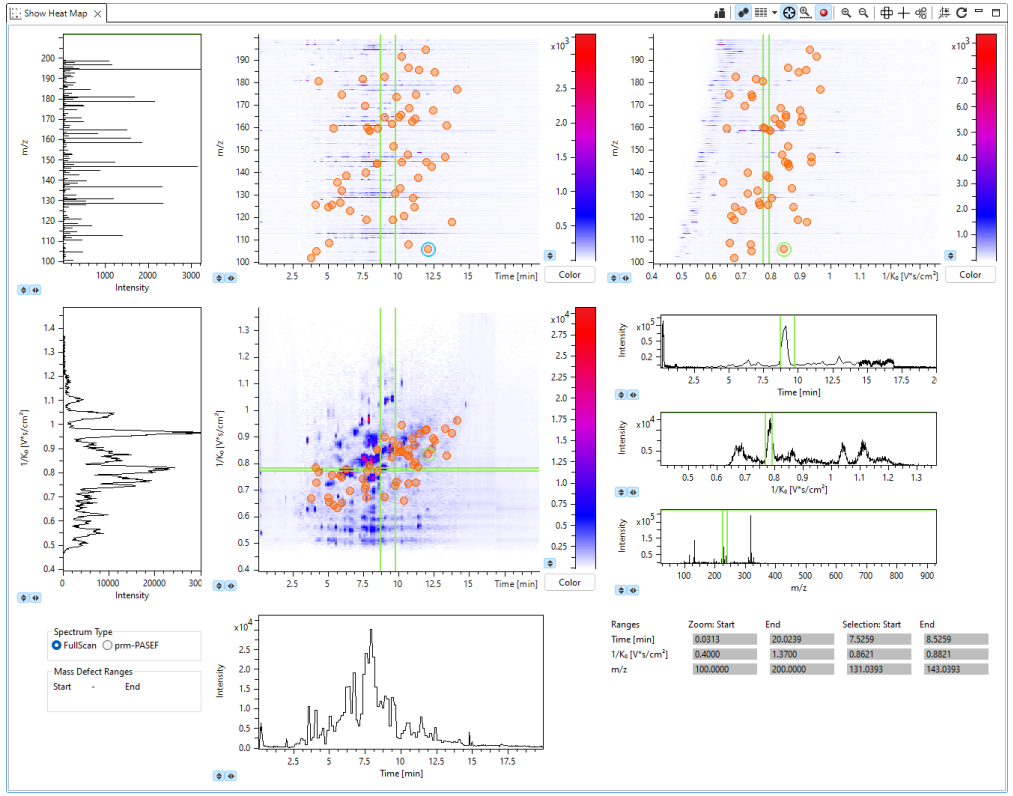


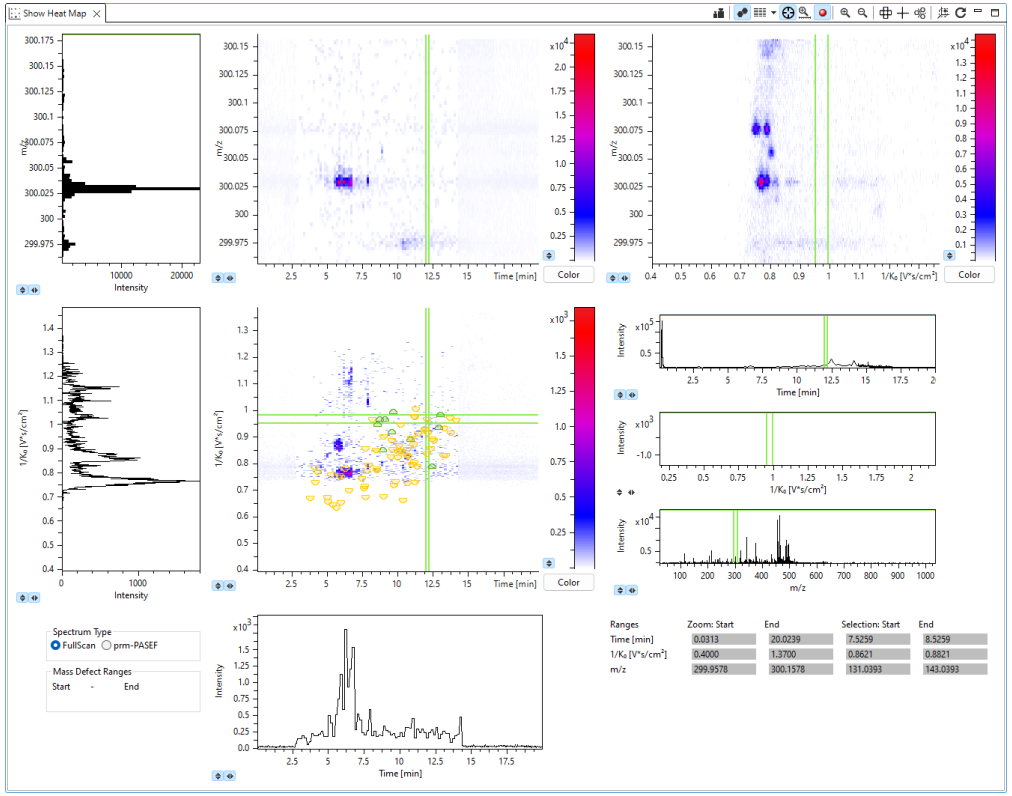




TASQ 2025b: HeatMap view

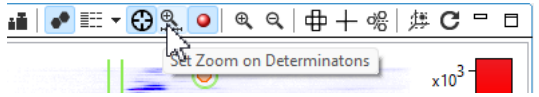
- Change z-Axis zoom with [CTRL]-LMB on a determination
- The respective z-axis coordinate will be changed to the z-value of selected determination +- offset





TASQ 2025b: HeatMap view

- Zoom in to show only bounding ranges of all determinations
- Zoom changes on selecting a determination
  - Create a sliced zoom with [Ctrl]-LMB on a determination
  - Move zoom range with [SHIFT]-LMB on a determination
- Edit zoom ranges and selection ranges manually

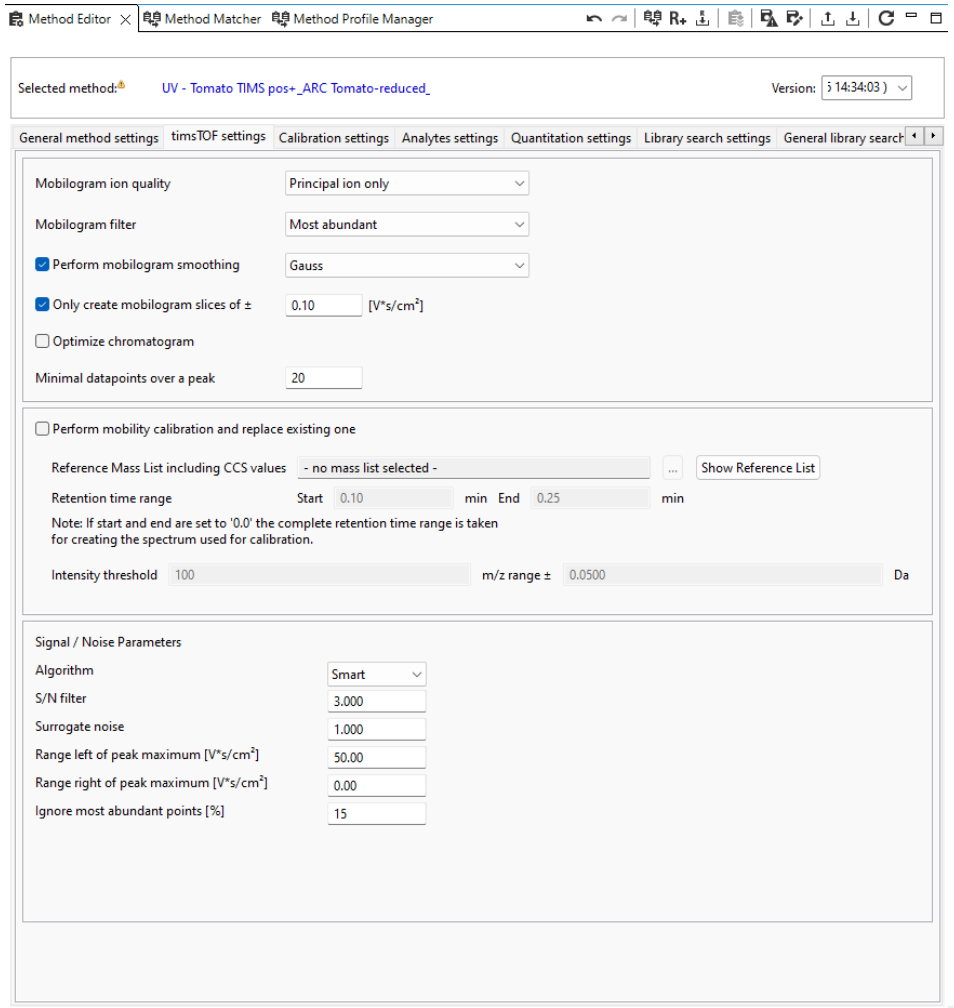


Ranges	Zoom: Start	End	Selection: Start	End
Time [min]	0.0313	20.0239	7.5259	8.5259
1/K₀ [V*s/cm²]	0.4000	1.3700	0.8621	0.8821
m/z	250	350	131.0393	143.0393

Ranges	Zoom: Start	End	Selection: Start	End
Time [min]	0.0313	20.0239	7.5259	8.5259
1/K₀ [V*s/cm²]	0.4000	1.3700	0.8621	0.8821
m/z	250	100	131.0393	143.0393

TASQ 2025b: TASQ Method Extensions for timsTOF Data Processing

- Added S/N threshold for mobilogram peak detection
- Optionally show Smart noise trace in mobilogram view
- Added minimum data points for mobilogram peak detection

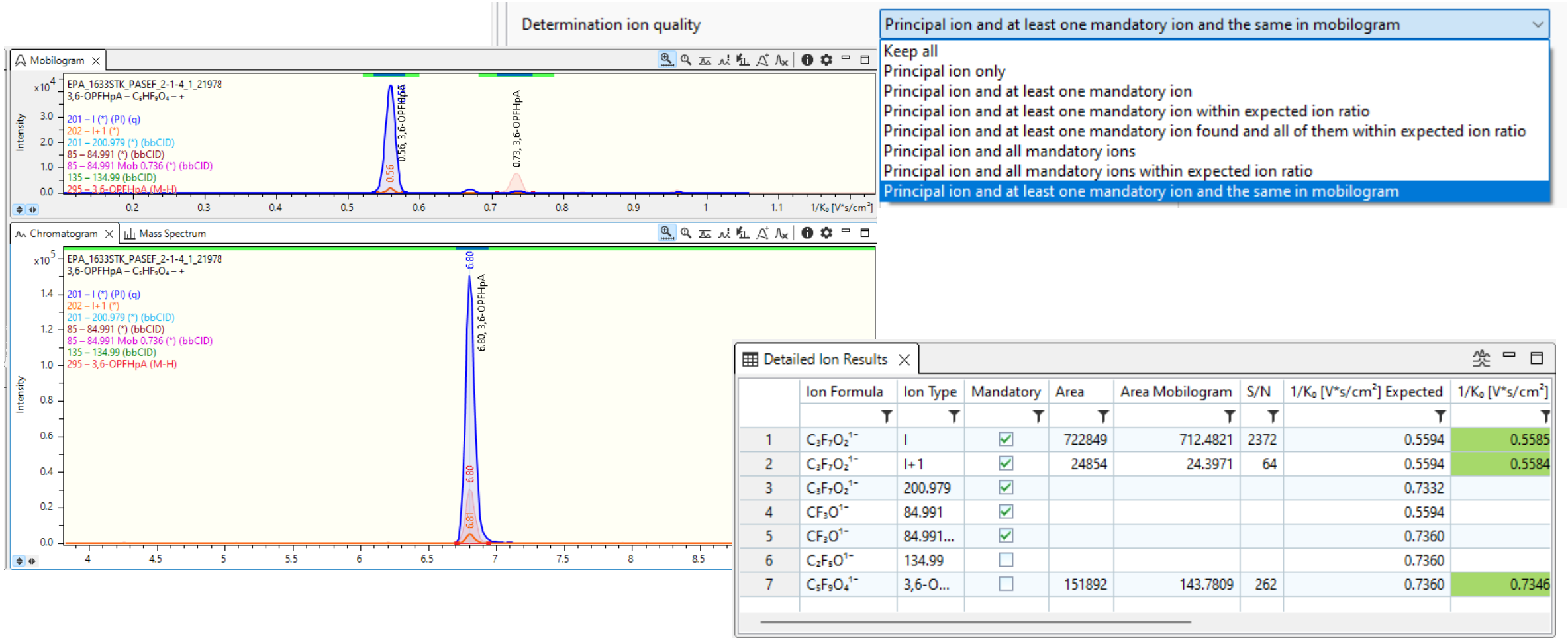


TASQ 2025B: Filter Options for Mobilogram Peak Assignment

- Determination ion quality:
  - New option: Principal ion and at least one mandatory ion and the same in mobilogram:
    - The principal ion and at least one mandatory ion must be detected on the chromatogram. In addition, for each chromatogram peak, the matching mobilogram peak must be found too. Otherwise, the determination will be discarded

- Mobilogram filter:
  - New option: Most mandatories and closest to CCS
    - The determination containing the principal ion (or any qualifier if not present) being closest to the expected CCS will remain
  - New option: Most mandatories and most abundant
    - The determination containing the principal ion (or any qualifier if not present) having the largest area will remain

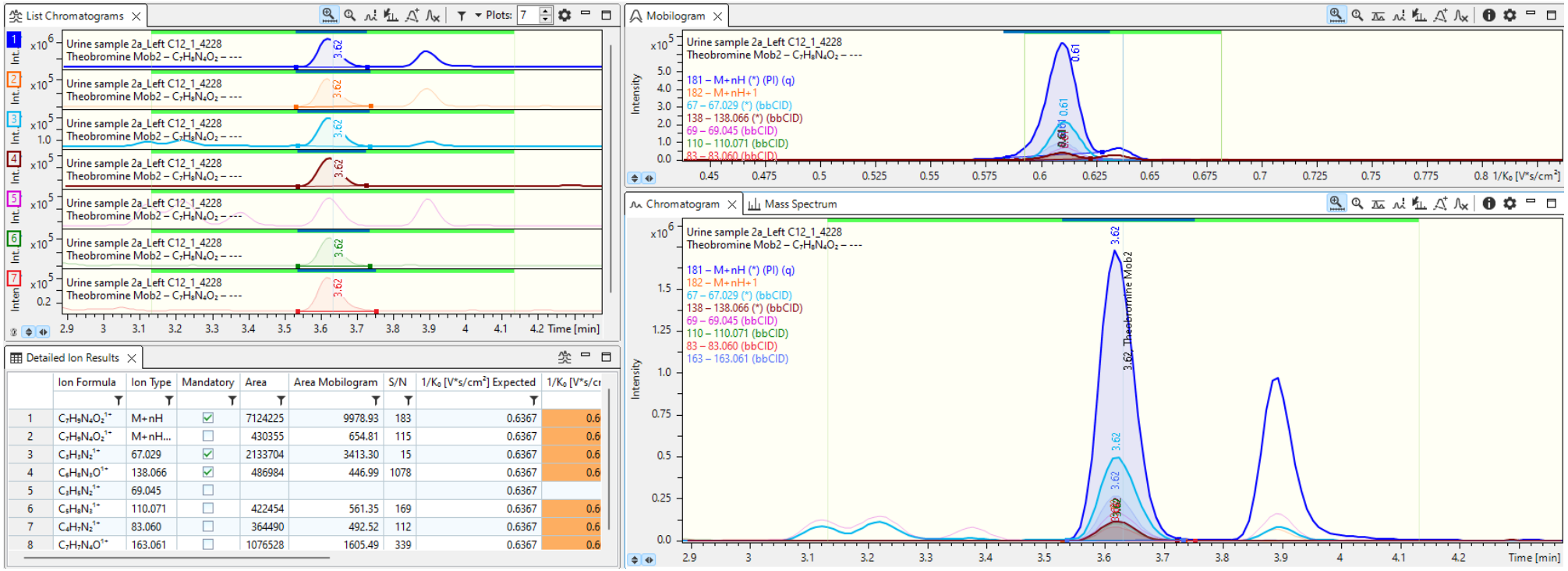
TASQ 2025b: Determination Filter: Principal Ion and at Least one Mandatory Ion in Chromatogram and Mobilogram



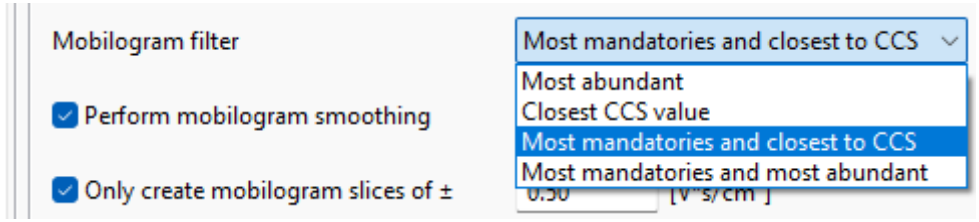
Detailed Ion Results

	Ion Formula	Ion Type	Mandatory	Area	Area Mobilogram	S/N	1/K₀ [V*s/cm²] Expected	1/K₀ [V*s/cm²]
1	$C_3F_7O_2^{1-}$	I	☑	722849	712.4821	2372	0.5594	0.5585
2	$C_3F_7O_2^{1-}$	I+1	☑	24854	24.3971	64	0.5594	0.5584
3	$C_3F_7O_2^{1-}$	200.979	☑				0.7332	
4	CF_3O^{1-}	84.991	☑				0.5594	
5	CF_3O^{1-}	84.991...	☑				0.7360	
6	$C_2F_5O^{1-}$	134.99	☐				0.7360	
7	$C_5F_9O_4^{1-}$	3,6-O...	☐	151892	143.7809	262	0.7360	0.7346

TASQ 2025b: Mobilogram Filter: Most Mandatories and Closest to CCS

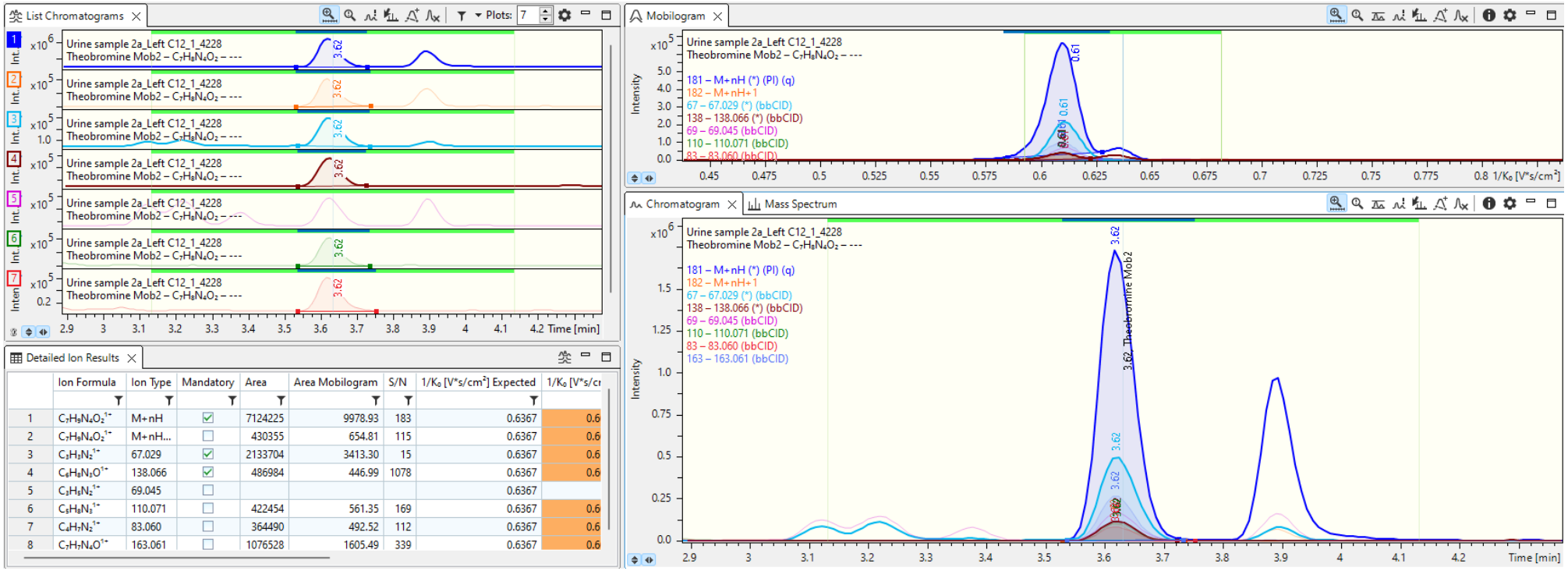


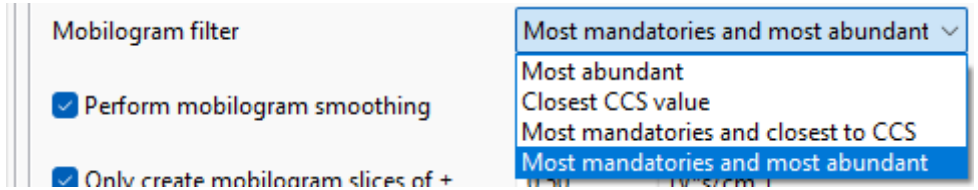
	Ion Formula	Ion Type	Mandatory	Area	Area Mobilogram	S/N	1/K₀ [V*s/cm²] Expected	1/K₀ [V*s/cm²
1	$C_7H_9N_4O_2^{1+}$	M+nH	☑	7124225	9978.93	183	0.6367	0.6
2	$C_7H_9N_4O_2^{1+}$	M+nH...	☐	430355	654.81	115	0.6367	0.6
3	$C_3H_3N_2^{1+}$	67.029	☑	2133704	3413.30	15	0.6367	0.6
4	$C_6H_8N_3O^{1+}$	138.066	☑	486984	446.99	1078	0.6367	0.6
5	$C_3H_3N_2^{1+}$	69.045	☐				0.6367	
6	$C_5H_8N_3^{1+}$	110.071	☐	422454	561.35	169	0.6367	0.6
7	$C_4H_7N_2^{1+}$	83.060	☐	364490	492.52	112	0.6367	0.6
8	$C_7H_7N_4O^{1+}$	163.061	☐	1076528	1605.49	339	0.6367	0.6



- The mobilogram peaks on the left hand side were choosen as there are more ions covered than with the peaks at the right hand side

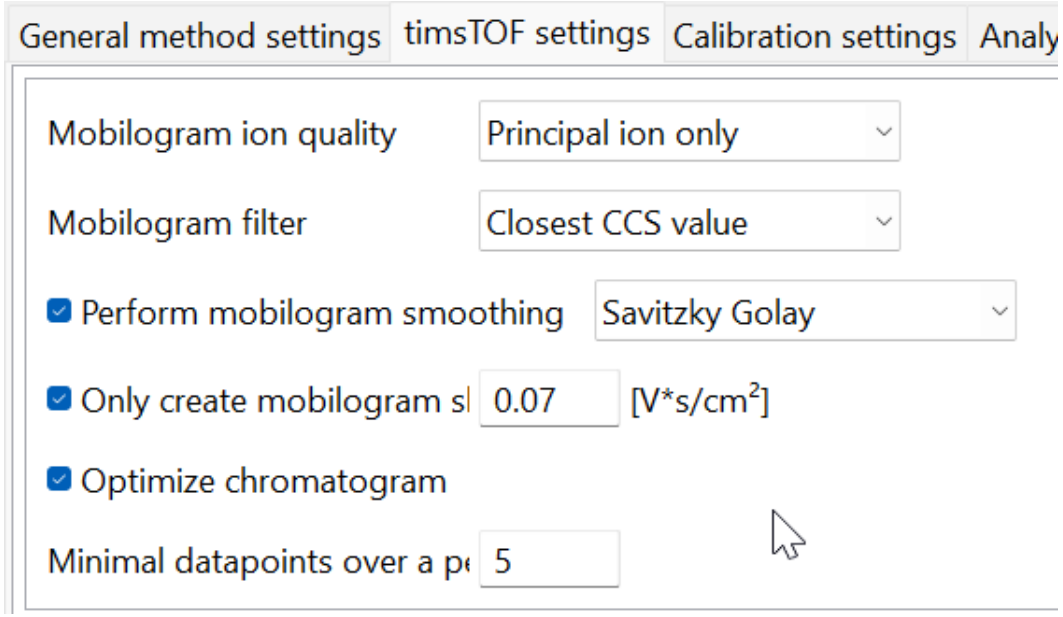
TASQ 2025b: Mobilogram Filter: Most Mandatories and most Abundant



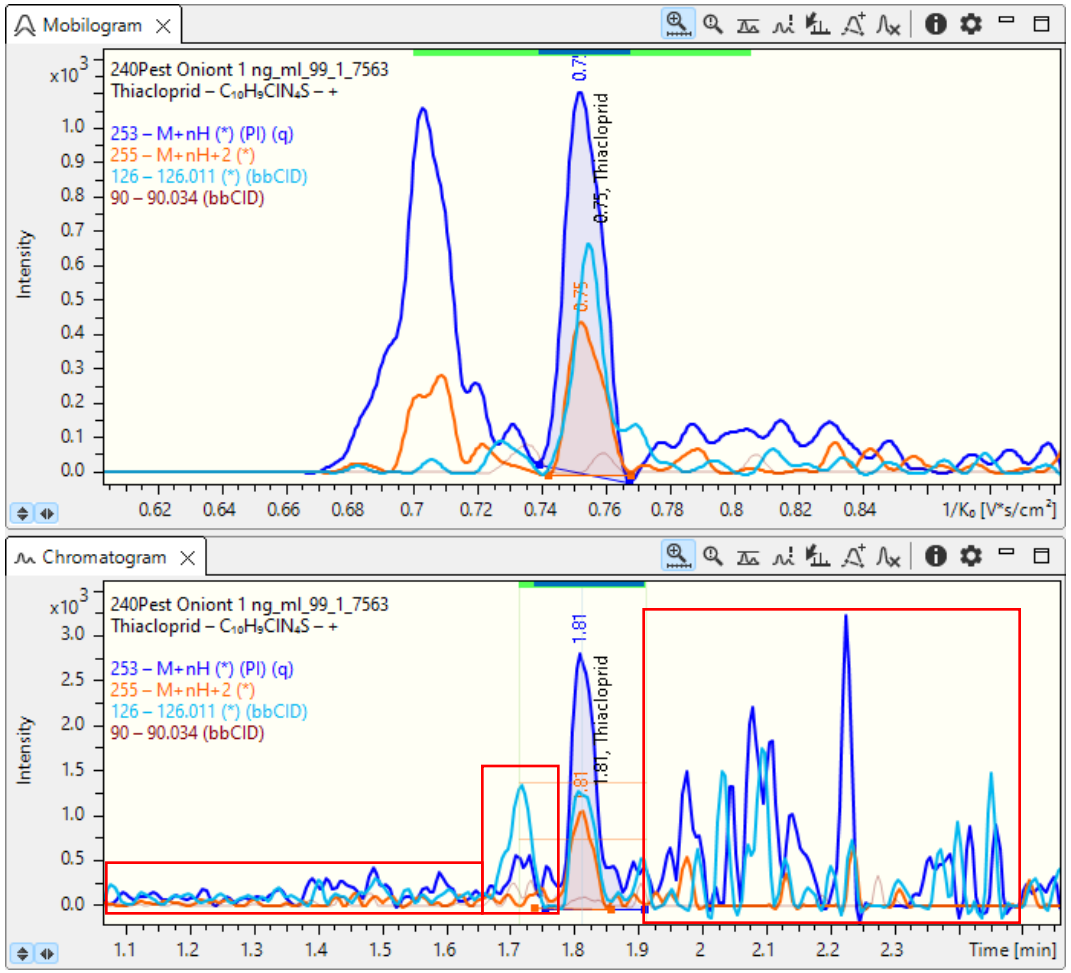


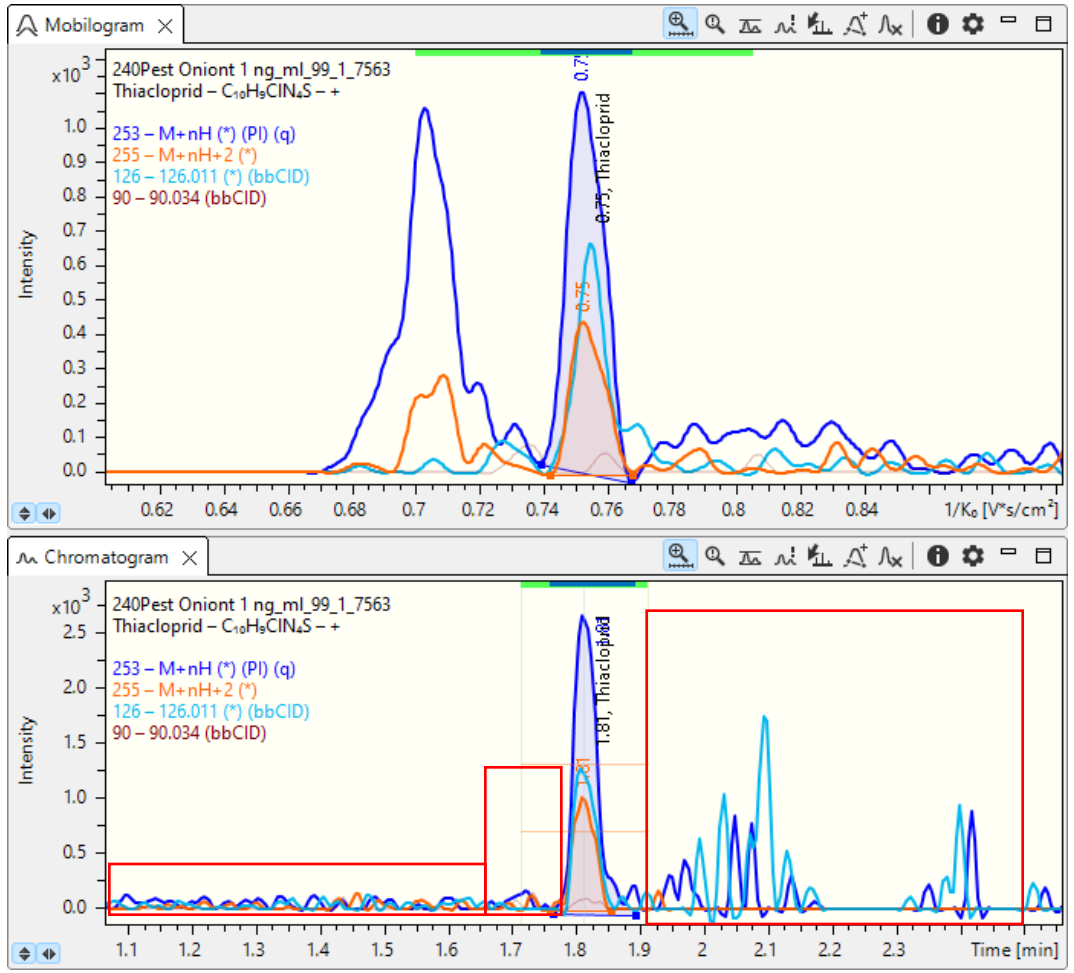
TASQ 2025b: Optimize Chromatogram

- In timsTOF settings a new parameter **Optimize chromatogram** is available
- After detection of mobilogram peak the EIC 1/K0 width will be adopted to the peak width of mobilogram peak

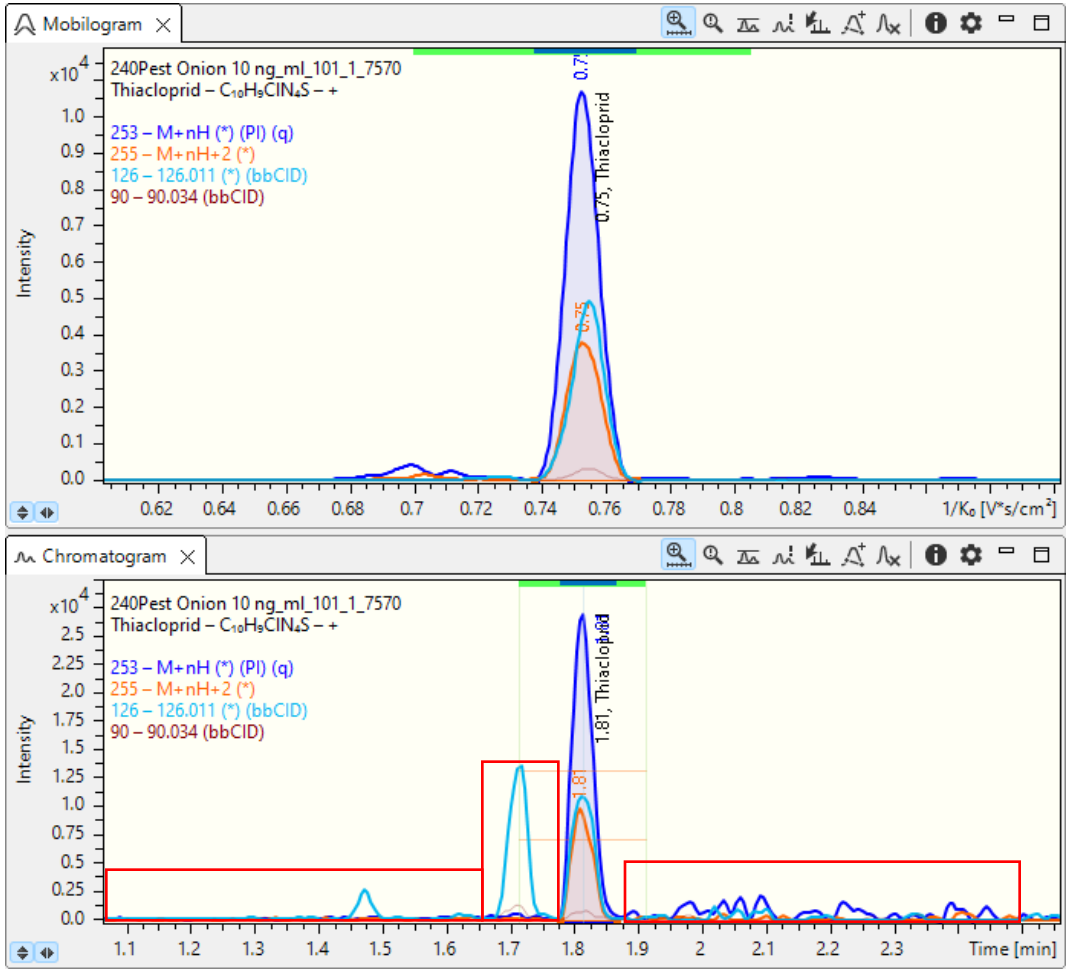


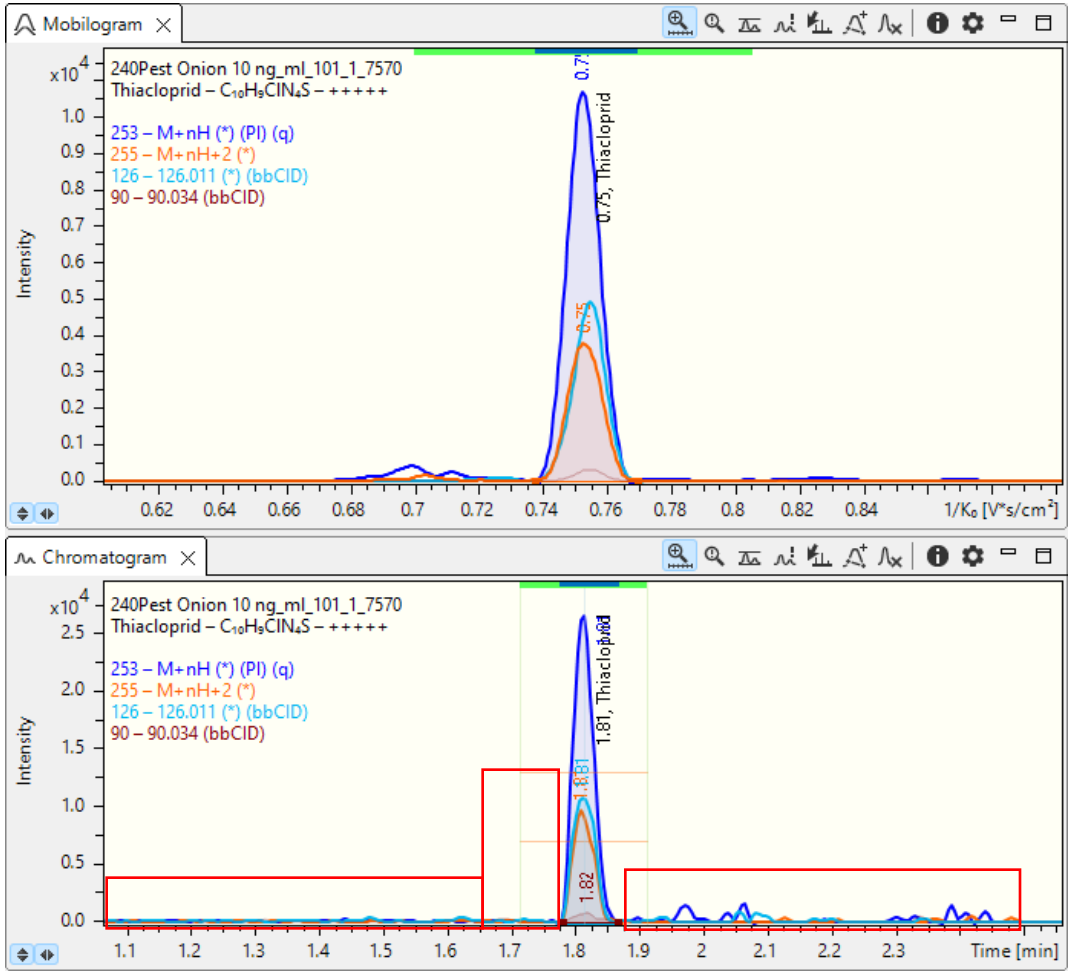
TASQ 2025b: Optimize Chromatogram – Thiacloprid 1 ng/mL





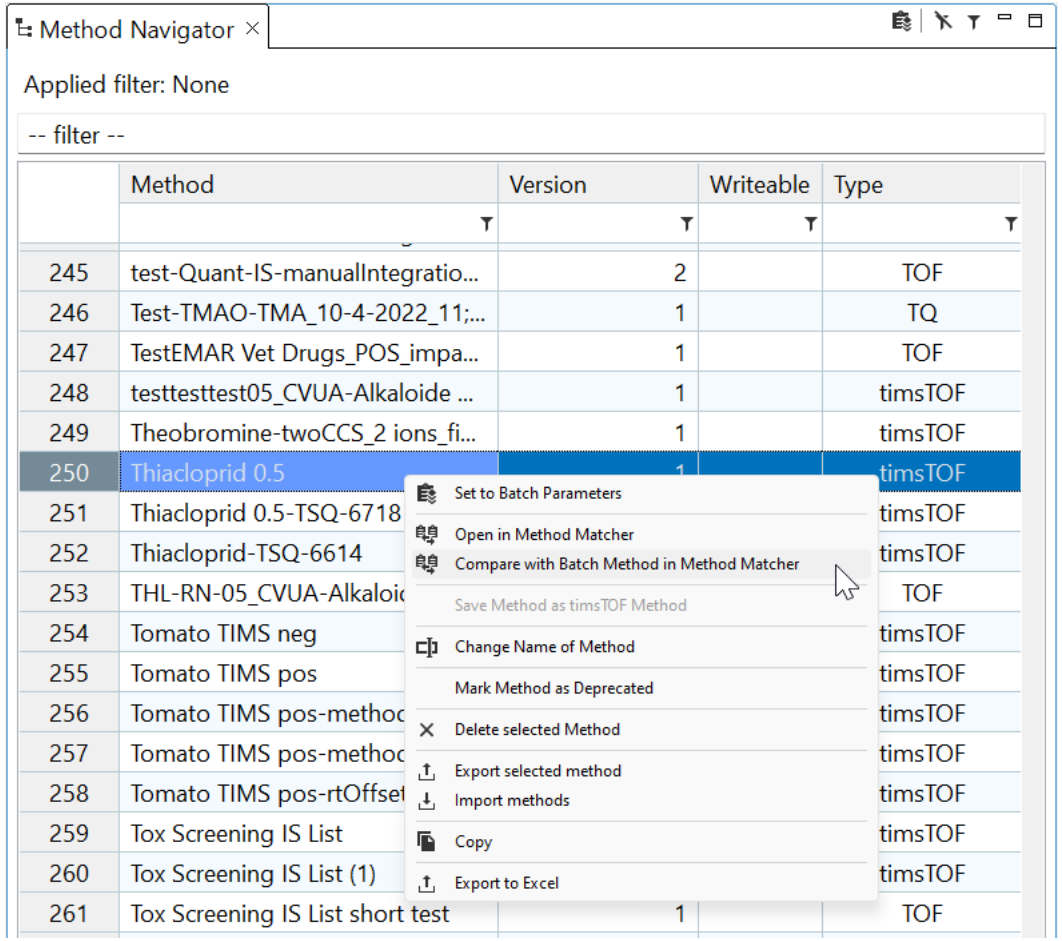
TASQ 2025b: Optimize Chromatogram – Thiacloprid 10 ng/mL





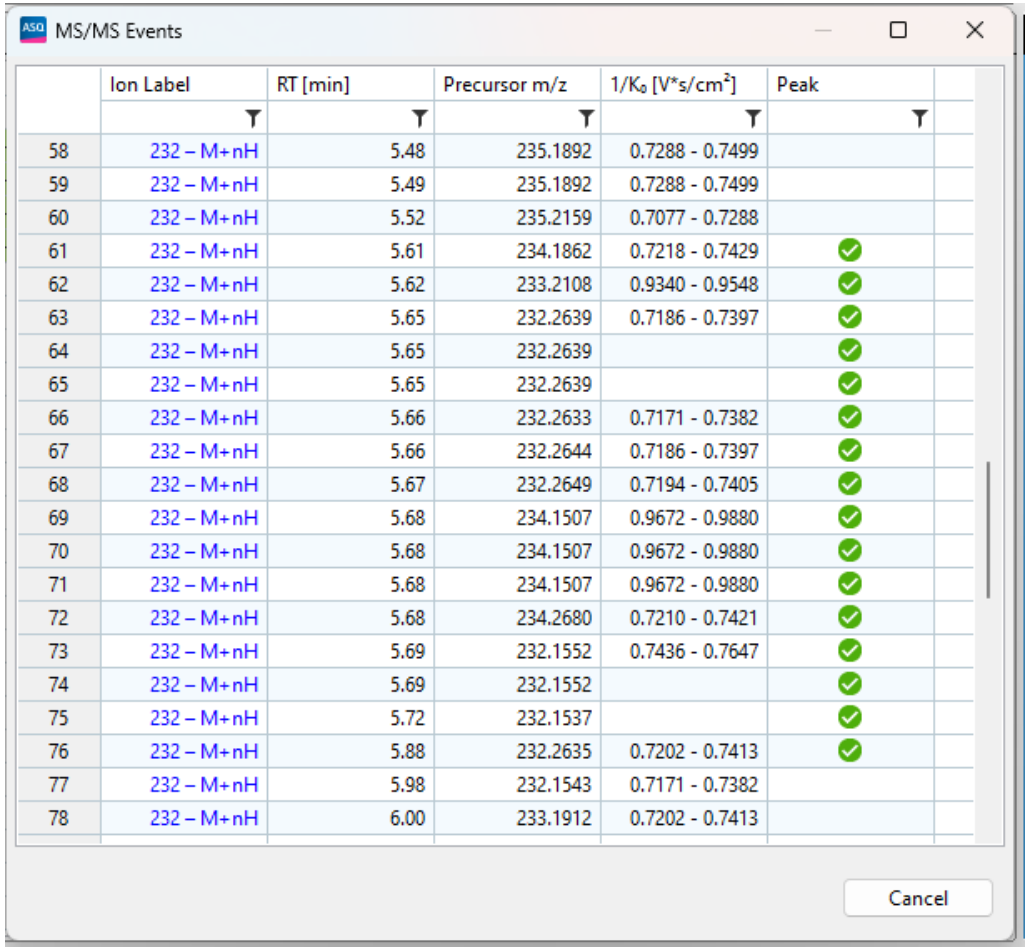
TASQ 2025b: Method Navigator – New Command Compare Batch Method with Selected Method

- Compare any method listed in the Method Navigator directly with the method assigned to the selected batch



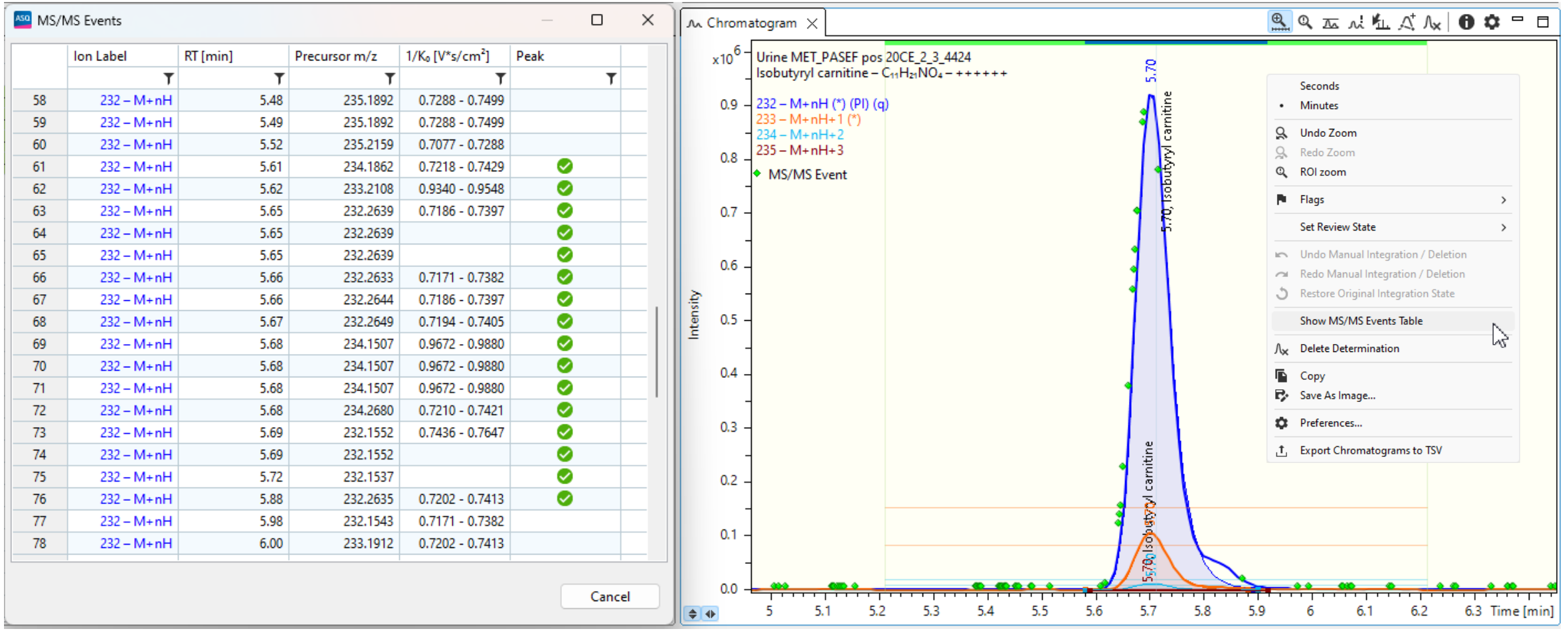
TASQ 2025b: Miscellaneous

- Show MS/MS events for selected determination
  - List all MS/MS events which matches to the ions specified for the respective analyte
  - In Chromatogram view call Show MS/MS events to review which MS/MS spectra are available
  - Enable MS/MS events option in Preferences>Chromatogram
  - Loading MS/MS events for a chromatogram takes some time and will be loaded each time the chromatogram view is updated (selection change)



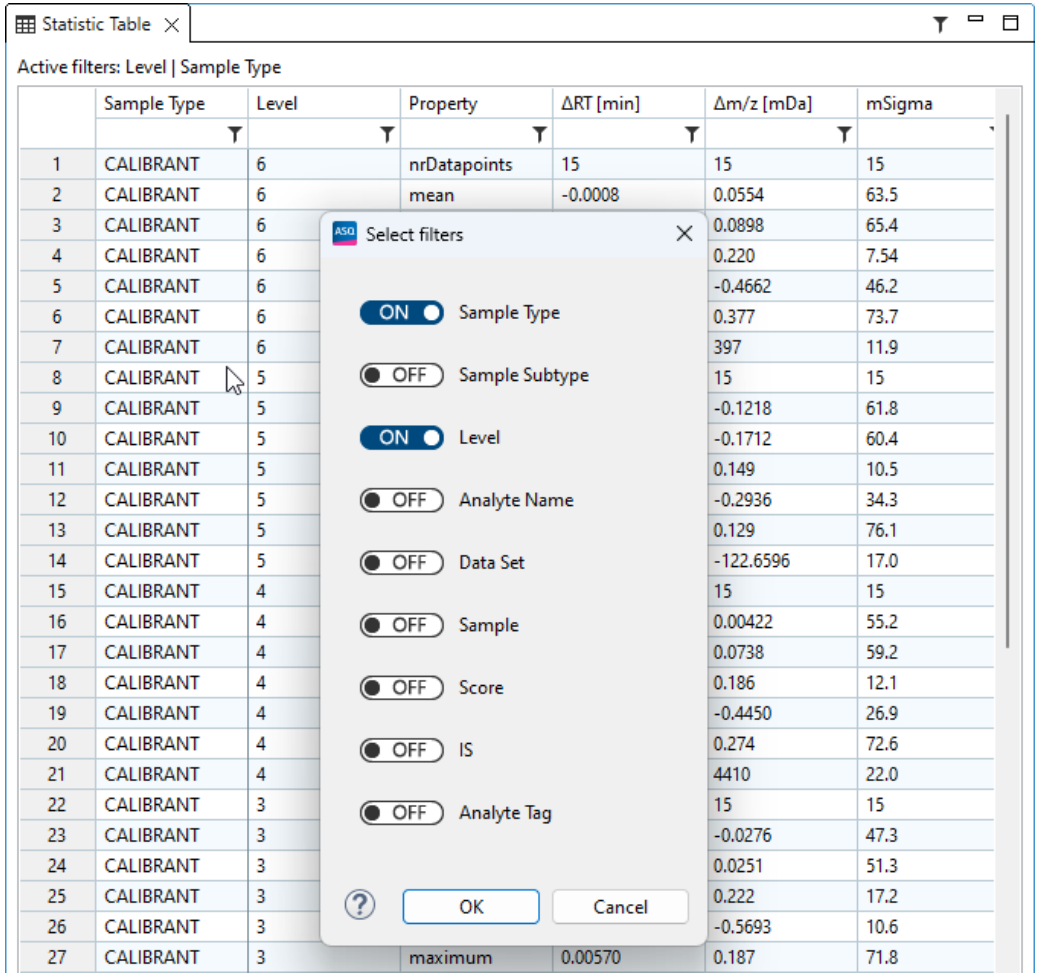
	Ion Label	RT [min]	Precursor m/z	1/K₀ [V*s/cm²]	Peak
58	232 – M+nH	5.48	235.1892	0.7288 - 0.7499	
59	232 – M+nH	5.49	235.1892	0.7288 - 0.7499	
60	232 – M+nH	5.52	235.2159	0.7077 - 0.7288	
61	232 – M+nH	5.61	234.1862	0.7218 - 0.7429	✓
62	232 – M+nH	5.62	233.2108	0.9340 - 0.9548	✓
63	232 – M+nH	5.65	232.2639	0.7186 - 0.7397	✓
64	232 – M+nH	5.65	232.2639		✓
65	232 – M+nH	5.65	232.2639		✓
66	232 – M+nH	5.66	232.2633	0.7171 - 0.7382	✓
67	232 – M+nH	5.66	232.2644	0.7186 - 0.7397	✓
68	232 – M+nH	5.67	232.2649	0.7194 - 0.7405	✓
69	232 – M+nH	5.68	234.1507	0.9672 - 0.9880	✓
70	232 – M+nH	5.68	234.1507	0.9672 - 0.9880	✓
71	232 – M+nH	5.68	234.1507	0.9672 - 0.9880	✓
72	232 – M+nH	5.68	234.2680	0.7210 - 0.7421	✓
73	232 – M+nH	5.69	232.1552	0.7436 - 0.7647	✓
74	232 – M+nH	5.69	232.1552		✓
75	232 – M+nH	5.72	232.1537		✓
76	232 – M+nH	5.88	232.2635	0.7202 - 0.7413	✓
77	232 – M+nH	5.98	232.1543	0.7171 - 0.7382	
78	232 – M+nH	6.00	233.1912	0.7202 - 0.7413	

TASQ 2025b: Show MS/MS Event on Chromatogram Traces



TASQ 2025b: Statistic Table

- Statistic Table improved setting of filters
- As more and more settings are added to the filters the toolbar took too much space and is wrapped if the view is too narrow
- Filter toolbar icon opens a dialog
- Selected filters are shown in the top left corner of view

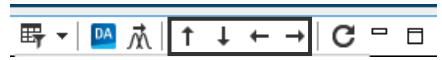


TASQ 2025b: Statistic Table, Statistic Graph, Batch Statistic Graph, RSD Statistic Graph

- All views shows the same set of numerical properties presented in the result tables
- All properties have the same label as known from result tables

TASQ 2025b: Miscellaneous

- Improvements on the presented tables in TASQ client
  - Tables does not jump on changes of data that often
  - Rearranged Filter options and improved presentation in UI
    - Open filter options dialog with [ALT]-F
- Clearer appearance of toolbars of result views
  - Removed arrow key to select next | previous determination or data set
  - Use arrow keys of keyboard instead

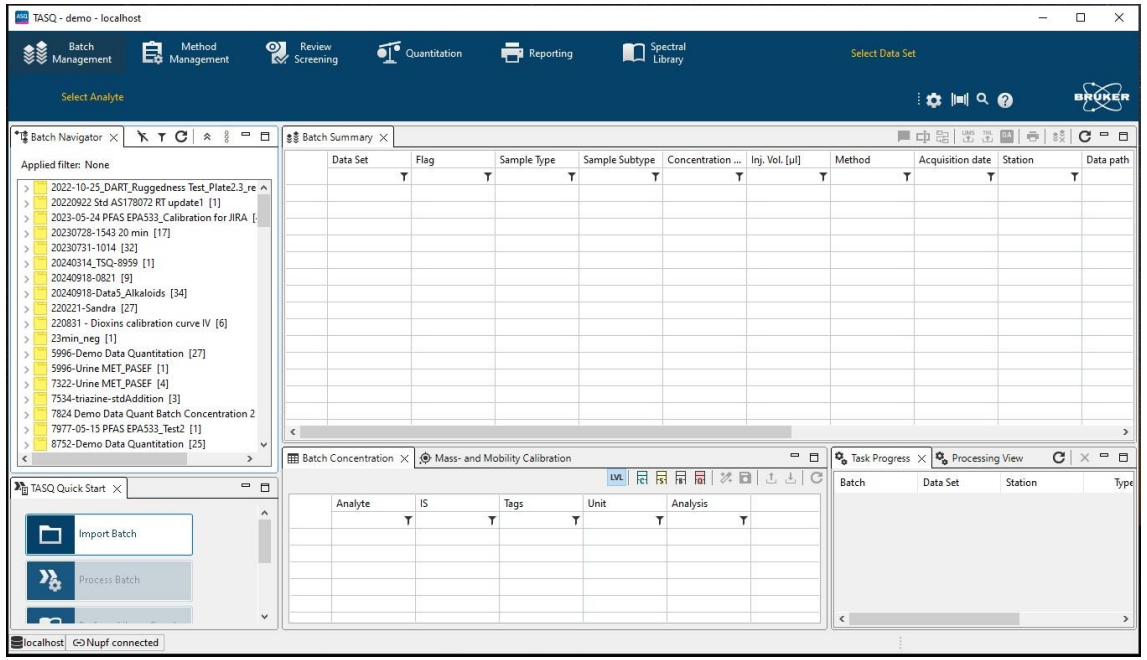


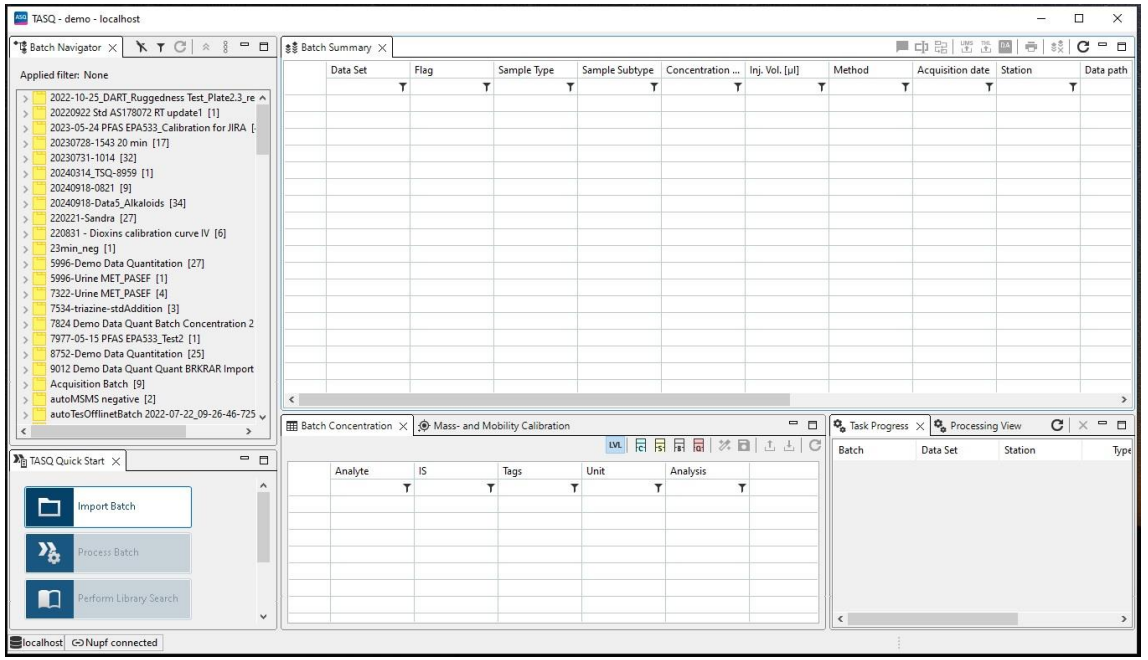
  - If a row is selected do not hide background colors

	Analyte Name	Quantity [ng/...	Score	Rule: RLE	RT Score	ΔRT [min]	RT expected [...	Ions Score	Exp.Diag.Ions	Found.Diag.Ions	Rule: Min R
1	Acetochlor	1.7	+++		++	-0.06	9.56	++	1	1	
2	Acibenzolar-S-...	4.5	+++		++	0.00	9.97	++	1	1	
3	Aclonifen	7.4	---		++	0.00	15.12	---	1	1	
4	Acrinathrin	19.1	+++		++	-0.09	20.30	++	1	1	
5	Alachlor	19.1	+++		++	-0.02	9.75	++	1	1	
6	Aldrin	18.6	+++		++	-0.08	10.92	++	1	1	
7	Allethrin I + II	n.a.	---		++	-0.09	12.15	---	1	1	

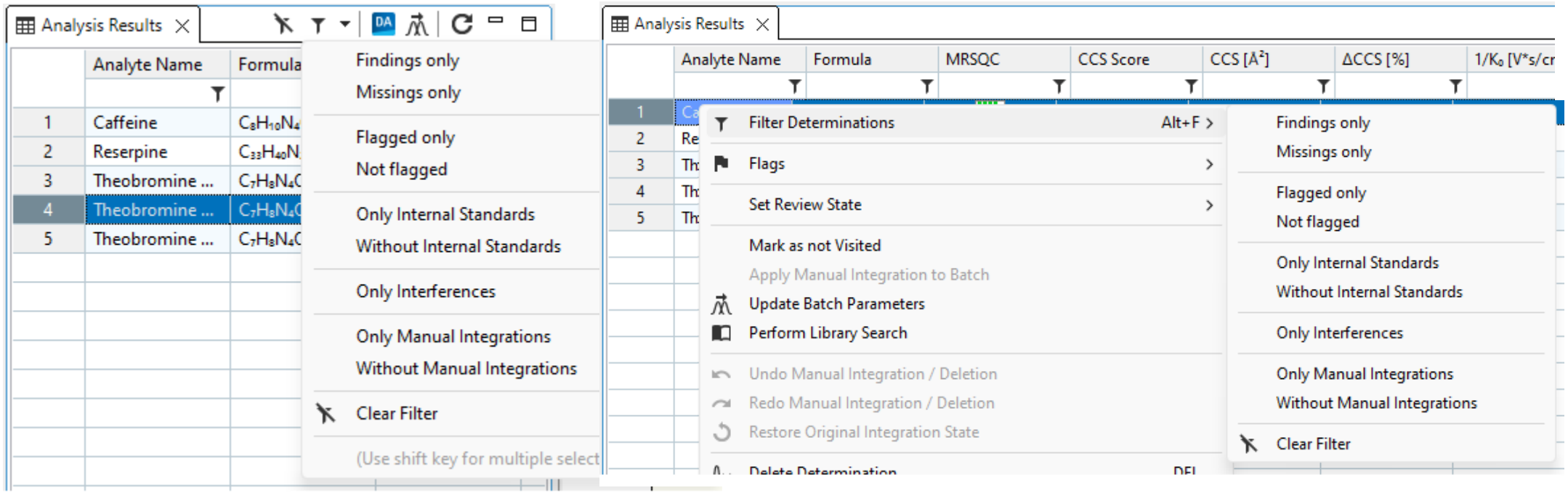
TASQ 2025b: Miscellaneous

- Toggle visibility of Bruker Ribbon on / off to save space by pressing F11 key, like internet browsers
  - Small devices with large display settings -> Bruker Ribbon will be shown in two or more lines as Icons have no space within one line

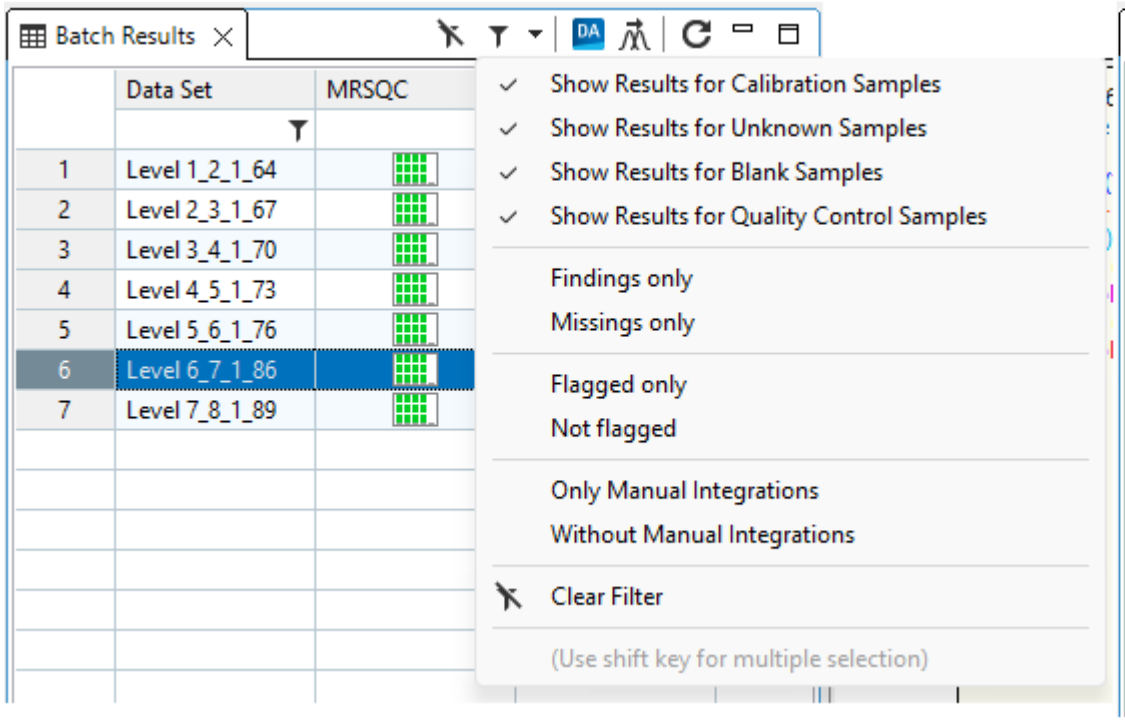


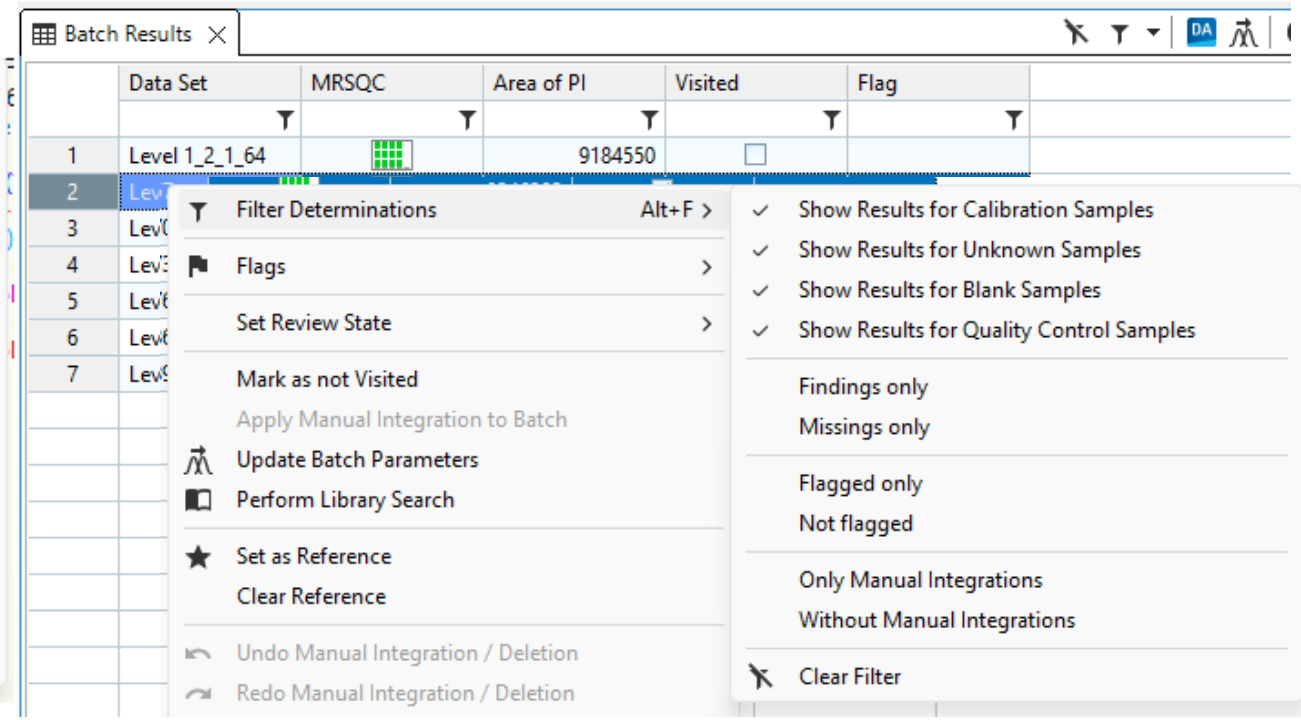


TASQ 2025b: Improved Filters for Analysis Results View



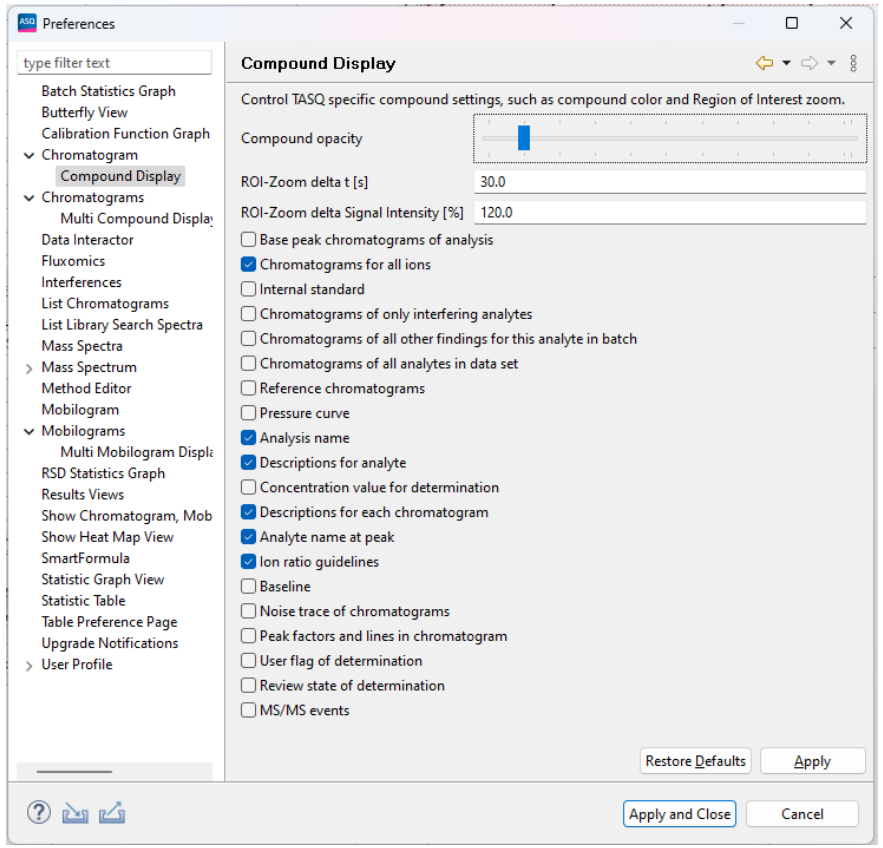
TASQ 2025b: Improved Filters for Batch Results View

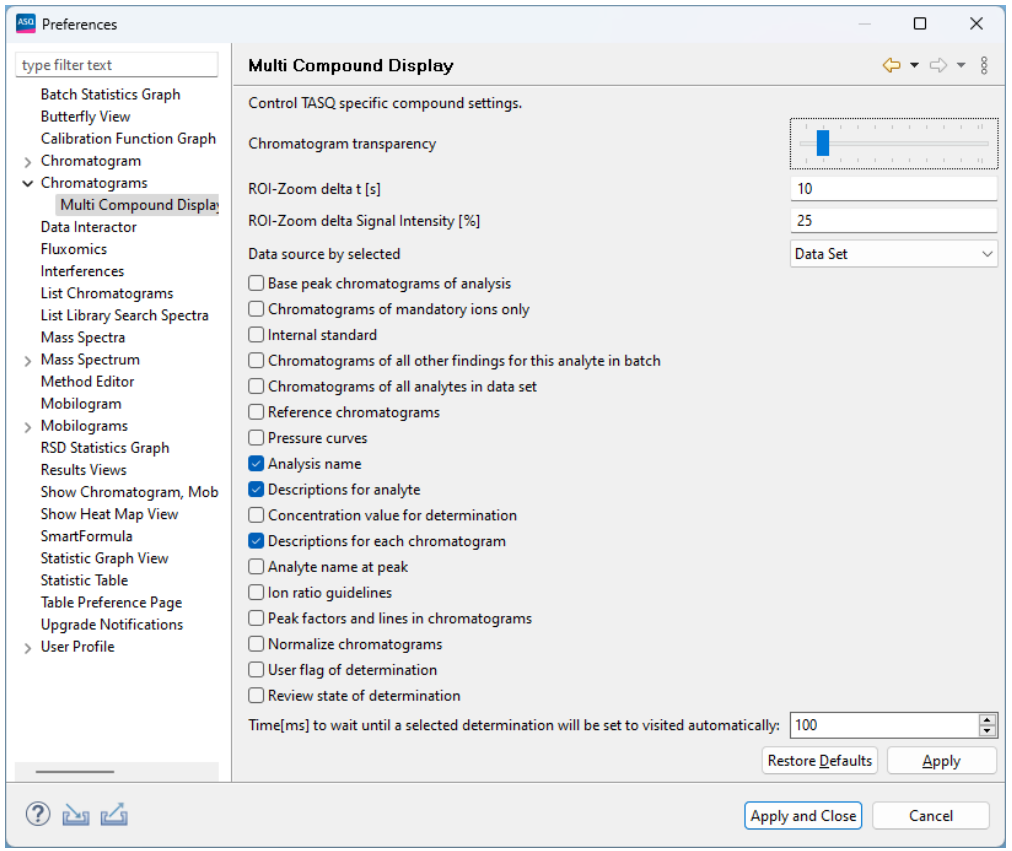




TASQ 2025b: Miscellaneous

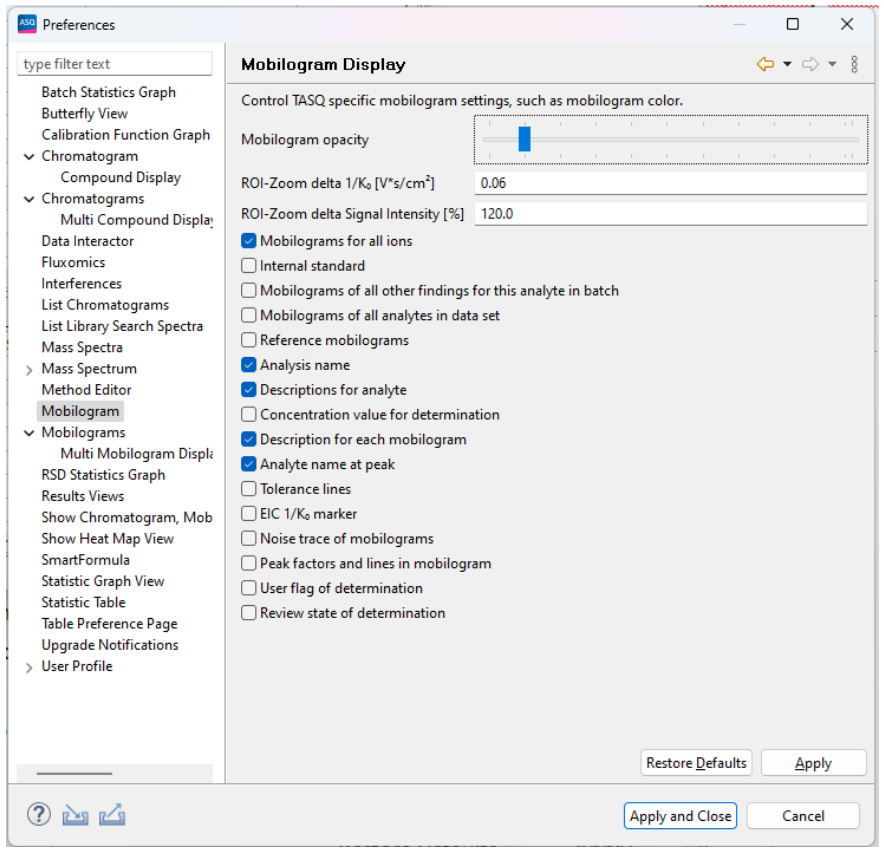
- Improved text and order of properties pages for Chromatogram, Chromatograms, Mobilogram, Mobilograms view

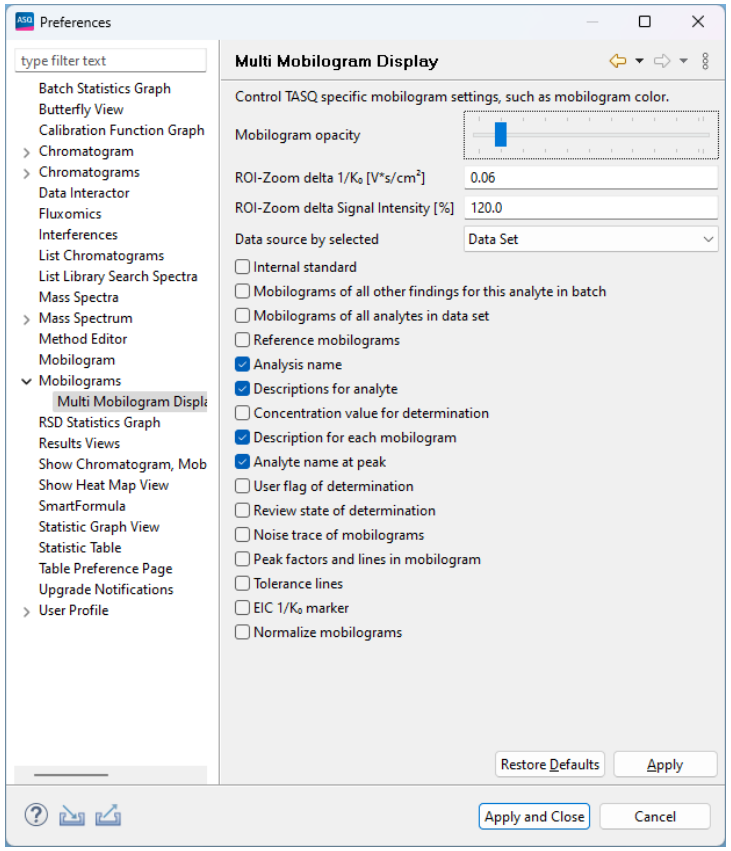




TASQ 2025b: Miscellaneous

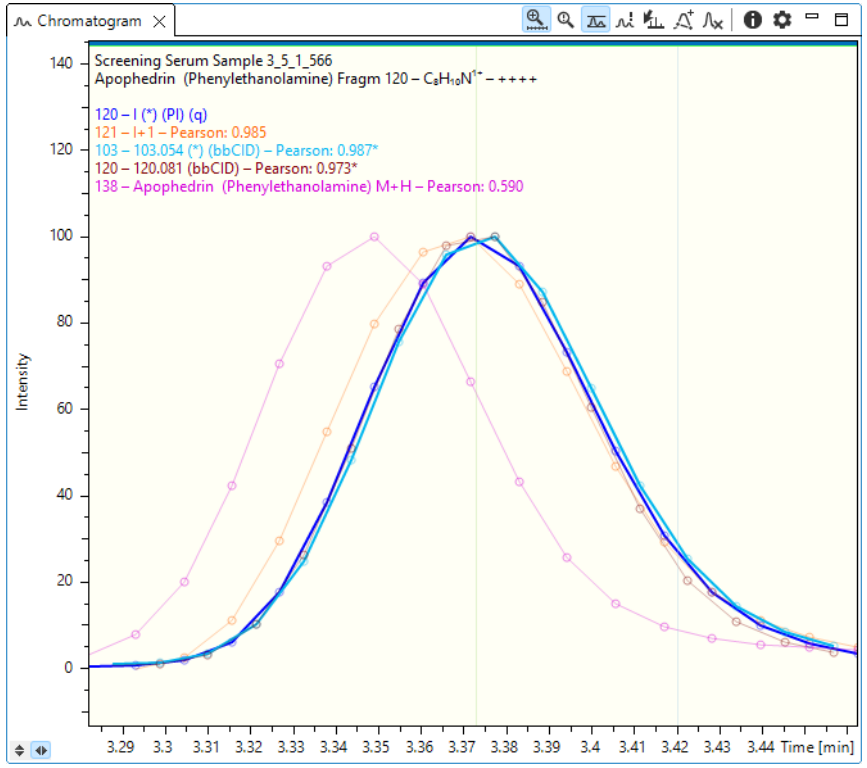
- Improved text and order of properties pages for Chromatogram, Chromatograms, Mobilogram, Mobilograms view

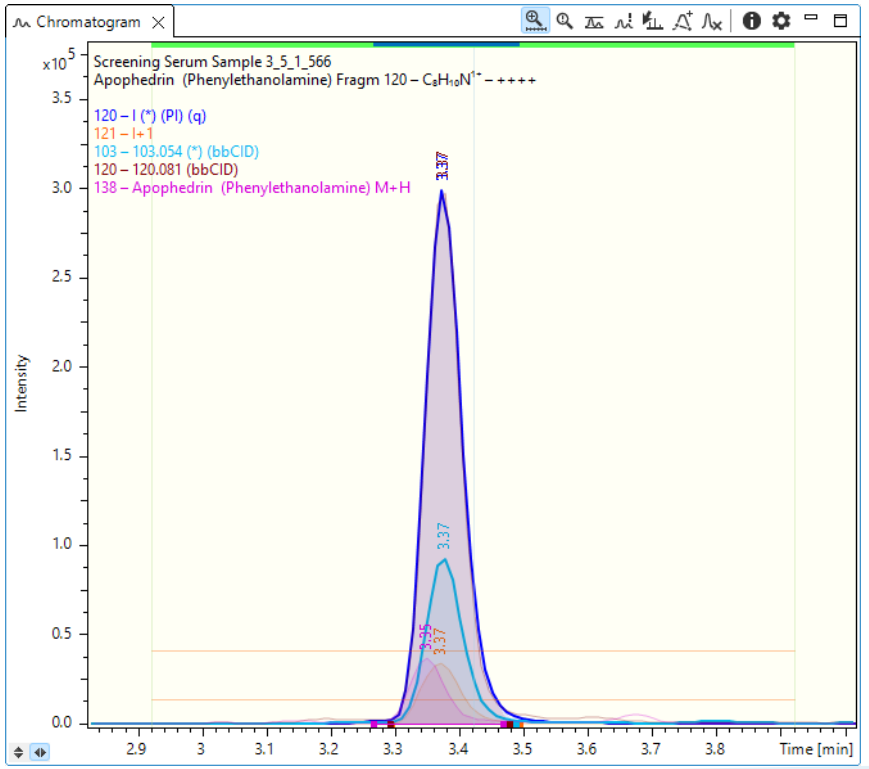




TASQ 2025b: Miscellaneous

- Calculate pearson correlation of chromatographic traces in Chromatogram view when normalizing chromatograms – does the different ions belong together or is this potentially a false positive?
- The traces are compared to the trace of the principle ion (PI), the correlation coefficient is added to the trace label



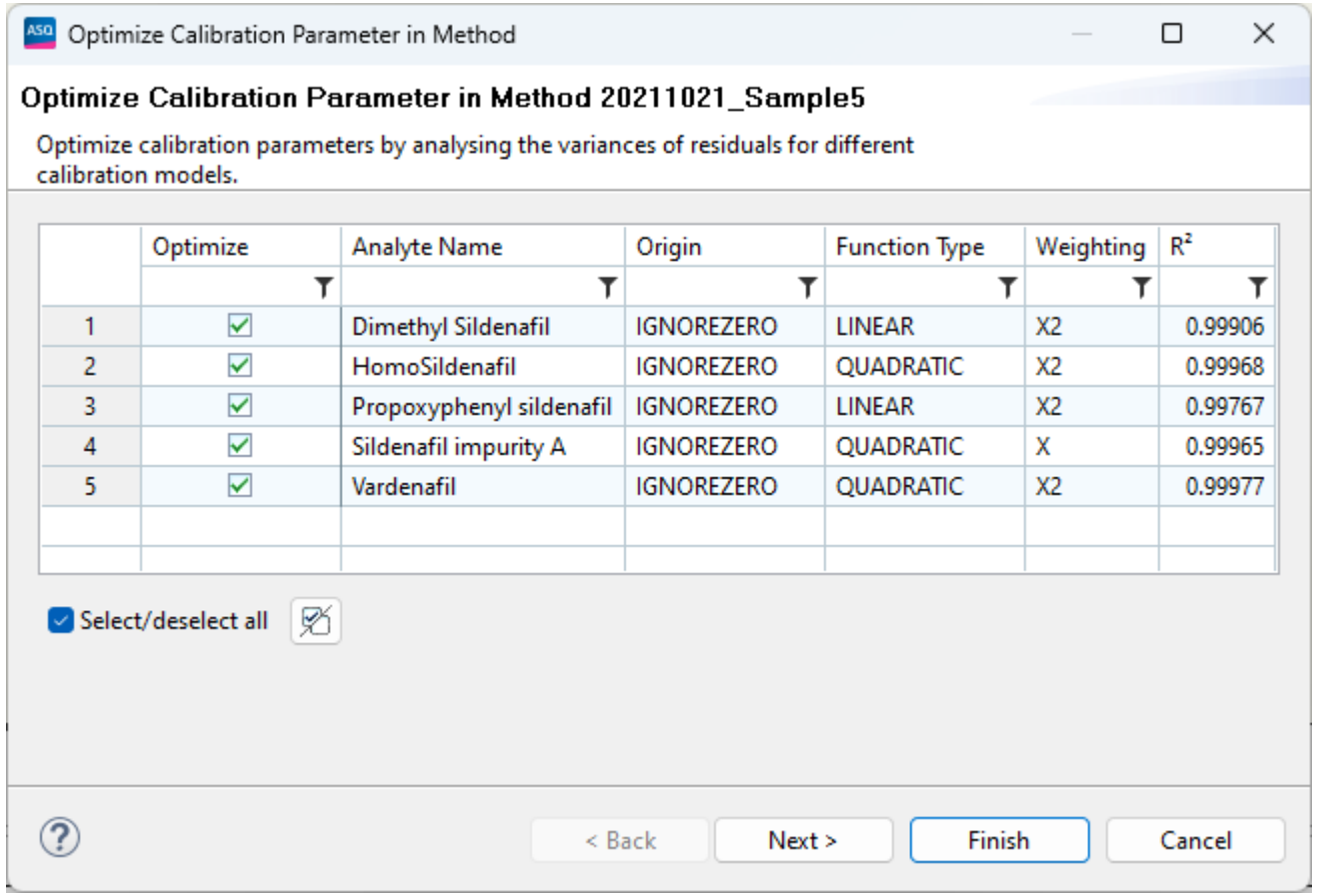


TASQ 2025b: Quantification

- New preference options for Calibration Function Graph view
  - Do not calculate automatically a calibration function for the selected analyte if the batch has not been quantified previously
  - Set the option for the regression calculation as specified in the TASQ method if calibration function has not been calculated previously
  - Use method settings for automatic generation of calibration functions in calibration function graph view if no calibration function is available
- Hint: If you want to know which is the best possible calibration function for the given data use Optimize Calibration Function to get the parameter settings for calculating the optimal calibration function
- Added command to set review state in Calibration Data Point view

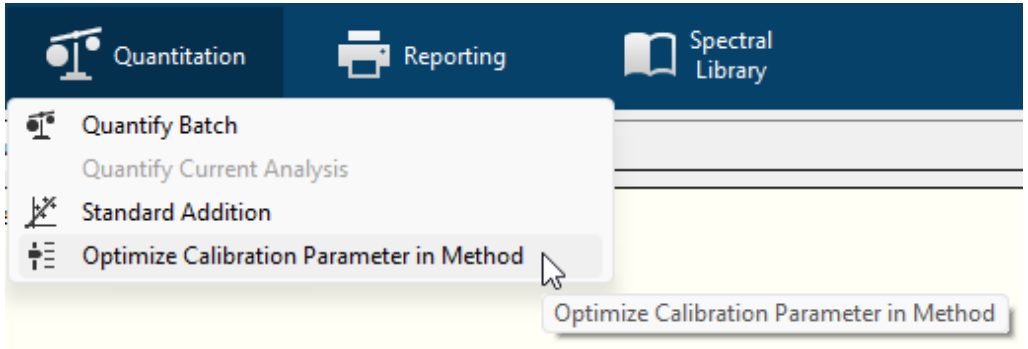
- Improvements to the Batch Concentrations view

TASQ 2025b: Hint Optimize Calibration Parameter in Method



	Optimize	Analyte Name	Origin	Function Type	Weighting	R^2
1	☑	Dimethyl Sildenafil	IGNOREZERO	LINEAR	X2	0.99906
2	☑	HomoSildenafil	IGNOREZERO	QUADRATIC	X2	0.99968
3	☑	Propoxyphenyl sildenafil	IGNOREZERO	LINEAR	X2	0.99767
4	☑	Sildenafil impurity A	IGNOREZERO	QUADRATIC	X	0.99965
5	☑	Vardenafil	IGNOREZERO	QUADRATIC	X2	0.99977

- Calculate the set of optimized parameters
- Check for heteroscedasticity
- Check which weighting / function type is best
- Transfer parameter sets to TASQ method
- Available from Quantitation menu



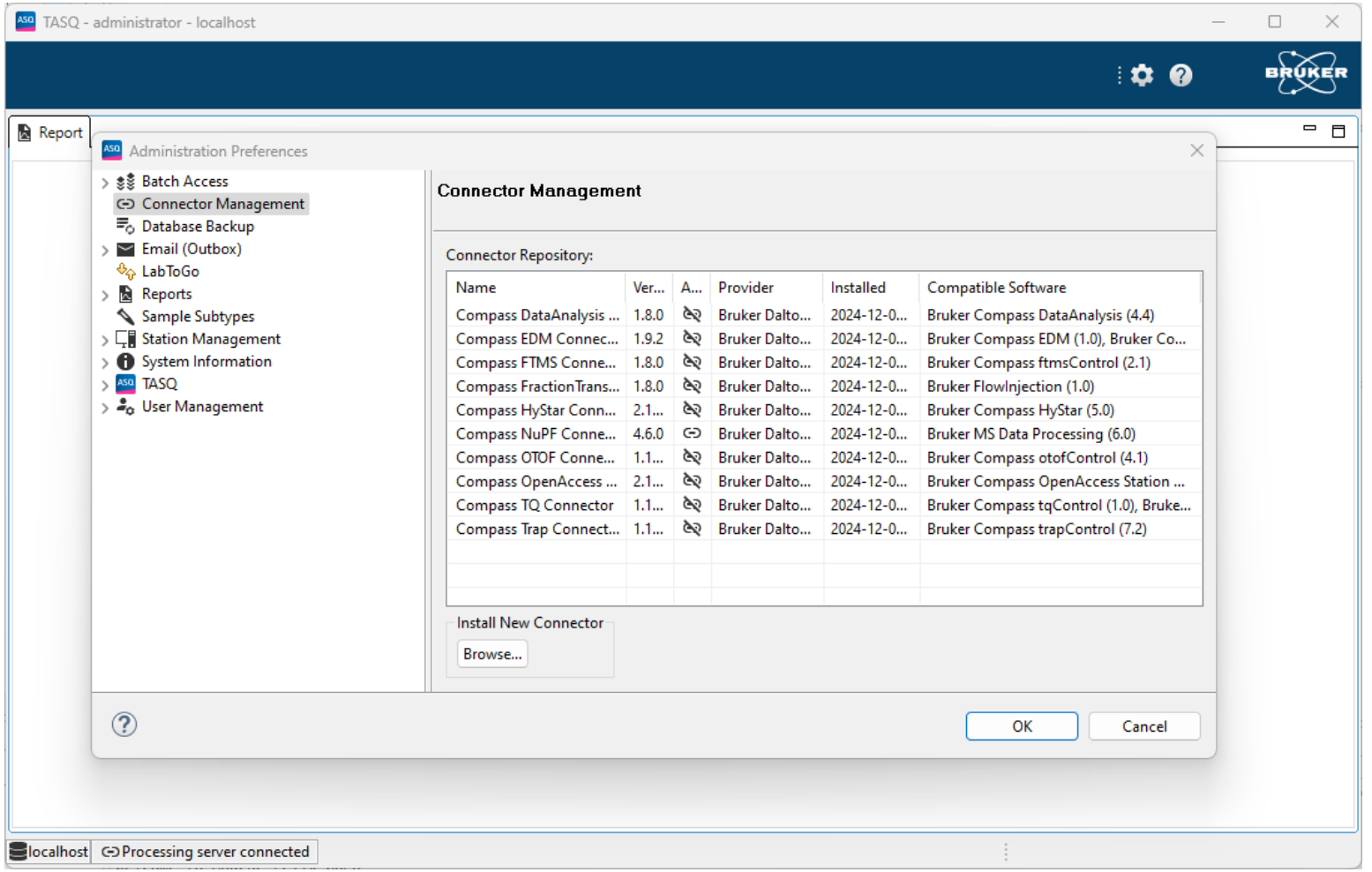
TASQ 2025b: Miscellaneus

- Support generation mobilograms for data sets with segments having different mobility ranges
- Enable manual integration with SHIFT LMB in mobilogram view, fix chromatogram view
- Improved Add Multiple Ions wizard: disable Finish button if not all mandatory properties are set (Spectrum type, charge state…)
- Reminder: In Butterfly view copy peak list of measured MS/MS spectrum or of library spectrum to clipboard Open Add Multiple Ions wizard in TASQ method editor to add multiple ions from peak list in clipboard to selected analyte

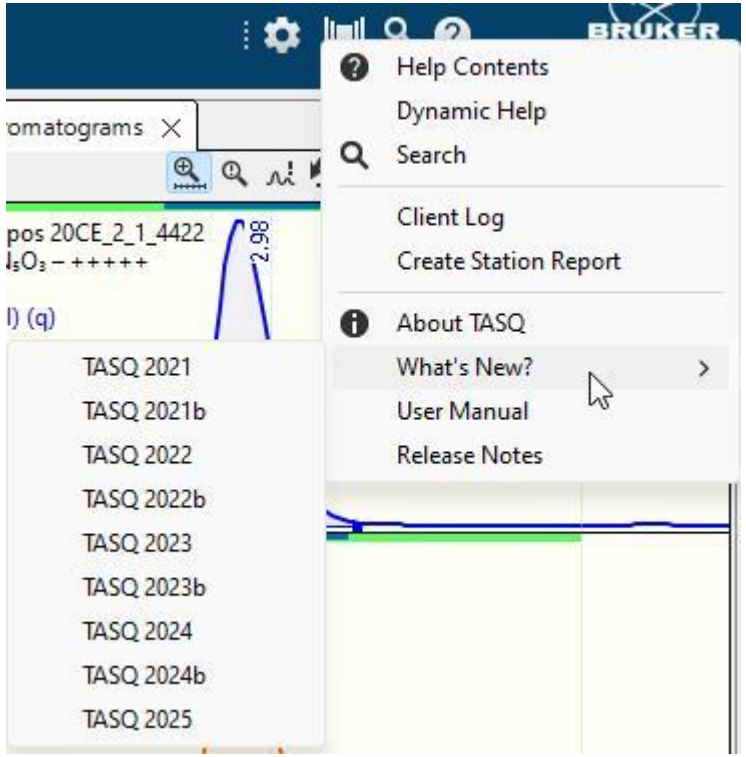
- Performance of installation of client and server components improved

TASQ 2025b: Connector Management Available in TASQ Administration Preferences

- If a user wants to import a brkrar file containing TQ methods into a TASQ only system EDM and TQ connectors have to be activated
- This can be done in connector management in Administration client or now in TASQ administration preferences



TASQ 2025b: Offer User Documentation within TASQ Help Menu

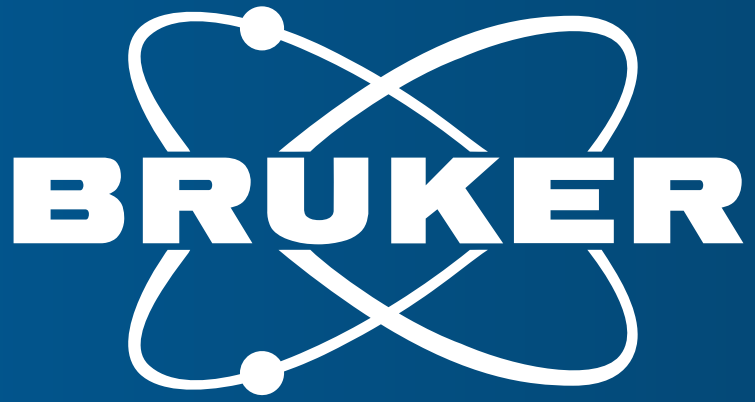


TASQ 2025b: Discontinued Feature

- Purity plot is no longer supported for Chromatogram/s, Mobilogram/s view

TASQ 2025b and older: Known Issues

- TSF data of autoMSMS data can‘t be processed by TASQ – no chromatograms can be created
  - TASQ is not able to retrieve the MS fullscan data
- This has been fixed in TASQ 2025b
- TASQ 2025: importing and processing of batches will show current date time of processing but the actual acquisition date in acquisition date column – fixed in TASQ 2025b
- On segment borders TQ instruments may store data which is non monotone – TASQ sorts data points by RT if it detects that time axis is not monotone



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