

What's new in TASQ 2023B

TASQ 2023B

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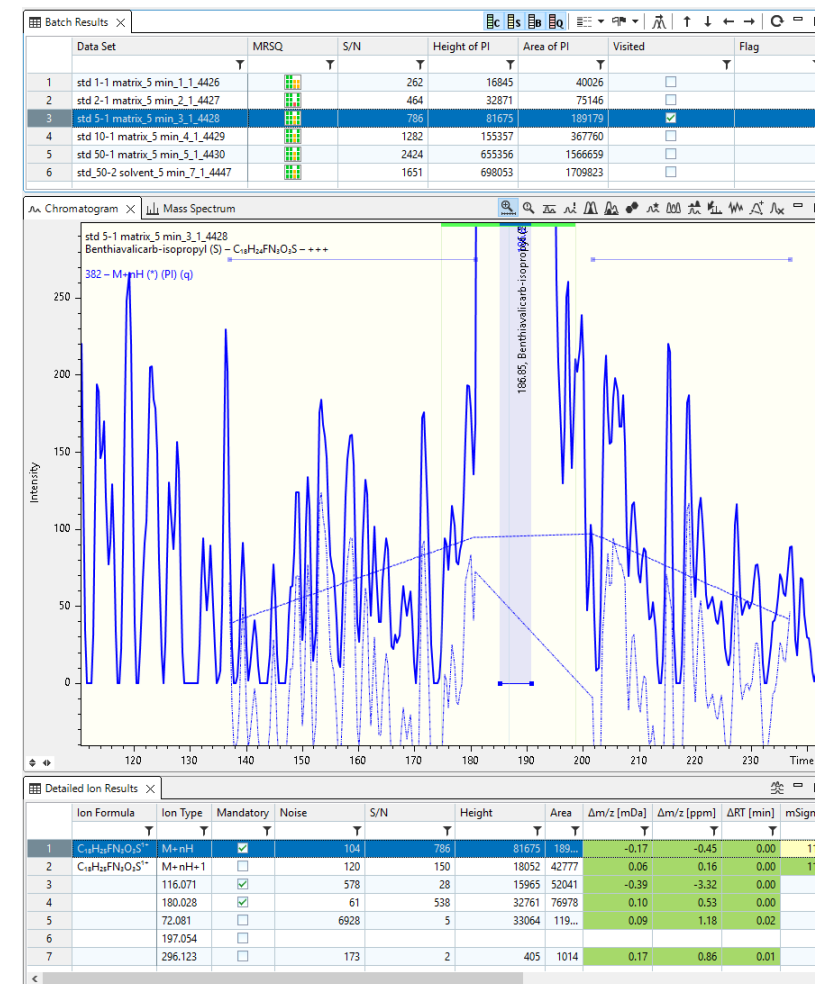
- Main Features
 - Additional noise calculation making use of an approach described by ASTM
 - Extension of Show Heat Map view
 - To show fullscan, bbCID, dia-PASEF data
 - To filter for mass defect ranges
 - Improved report data provider to include missings for showing results of one analyte in the entire batch
 - New report data provider to retrieve list of tags of analytes in a TASQ method
 - New batch statistics graph report data provider
 - Information based on raw data shown in TASQ RealTimeQC
 - More elaborated highlighting of outliers in TASQ RealTimeQC

What's new TASQ 2023B

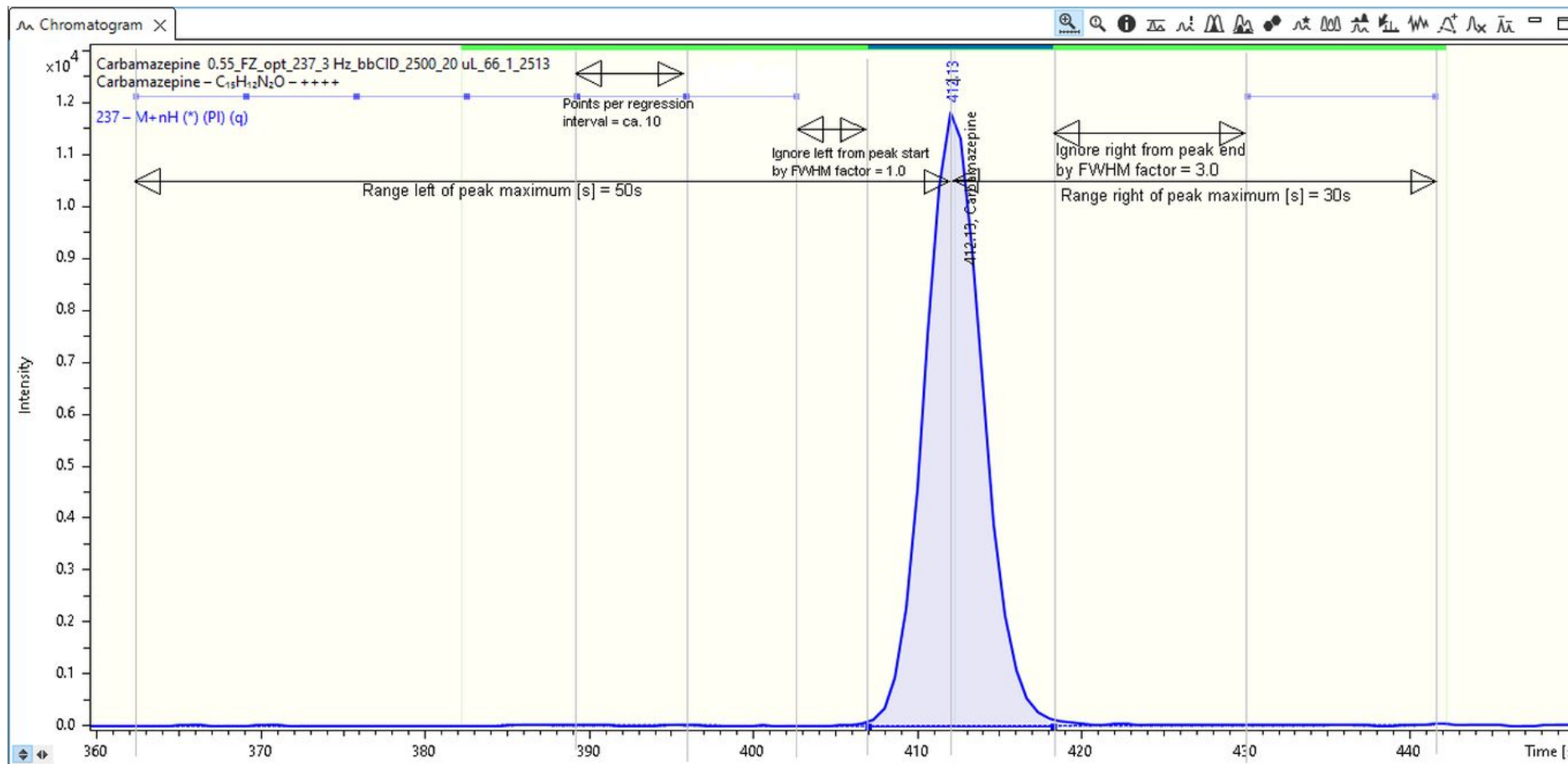
- Minor improvements
 - Changes due to improved corporate design
 - TASQ 2023B can inform whether newer SW versions are available
 - More detailed information in chromatogram, mobilogram, and MS spectrum view on how the shown data was created
 - Peak asymmetry information shown in Chromatogram and Mobilogram view
 - Improved handling of perspectives
 - Import / export perspective definitions
 - Assign user defined perspectives to Bruker Ribbon bar

New Noise Estimation

- Thorough evaluation of noise/background estimation required
- Decision needed which parameter shall be exposed in the TASQ method
- Add new option for surrogate noise if noise can't be calculated to be added in TASQ method
- Heuristics:
 - Traces are segmented.
 - In each segment a linear regression is calculated
 - Residuals of regression are considered to be noise/background
 - Peak of interest is excluded
 - Remaining intensities top 80 – 100 % are considered as signal
 - A peak detection may exclude intense peaks
 - Remaining signals are used for noise/background estimation



Parameters for new Noise Algorithm



Signal / Noise Parameters	
Algorithm	Smart
S/N filter	1.000
Surrogate noise	1.000
Ignore most abundant points [%]	15
Ignore left from peak start by FWHM factor	1.00
Ignore right from peak end by FWHM factor	3.00
Range left of peak maximum [s]	50.00
Range right of peak maximum [s]	30.00
Points per regression interval	10

Parameters for new Noise Algorithm

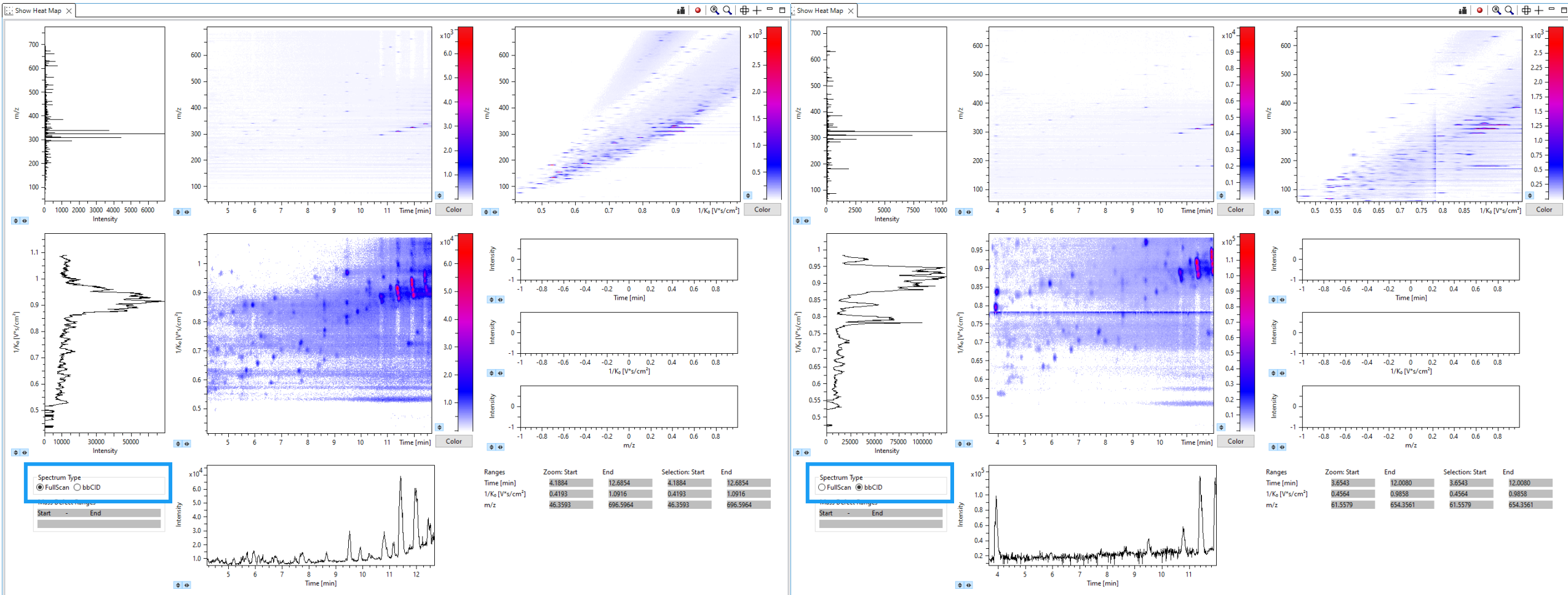
User can choose from three settings

Signal / Noise Parameters	
Algorithm	Classic ▾
S/N filter	3.000
Surrogate noise	1.000

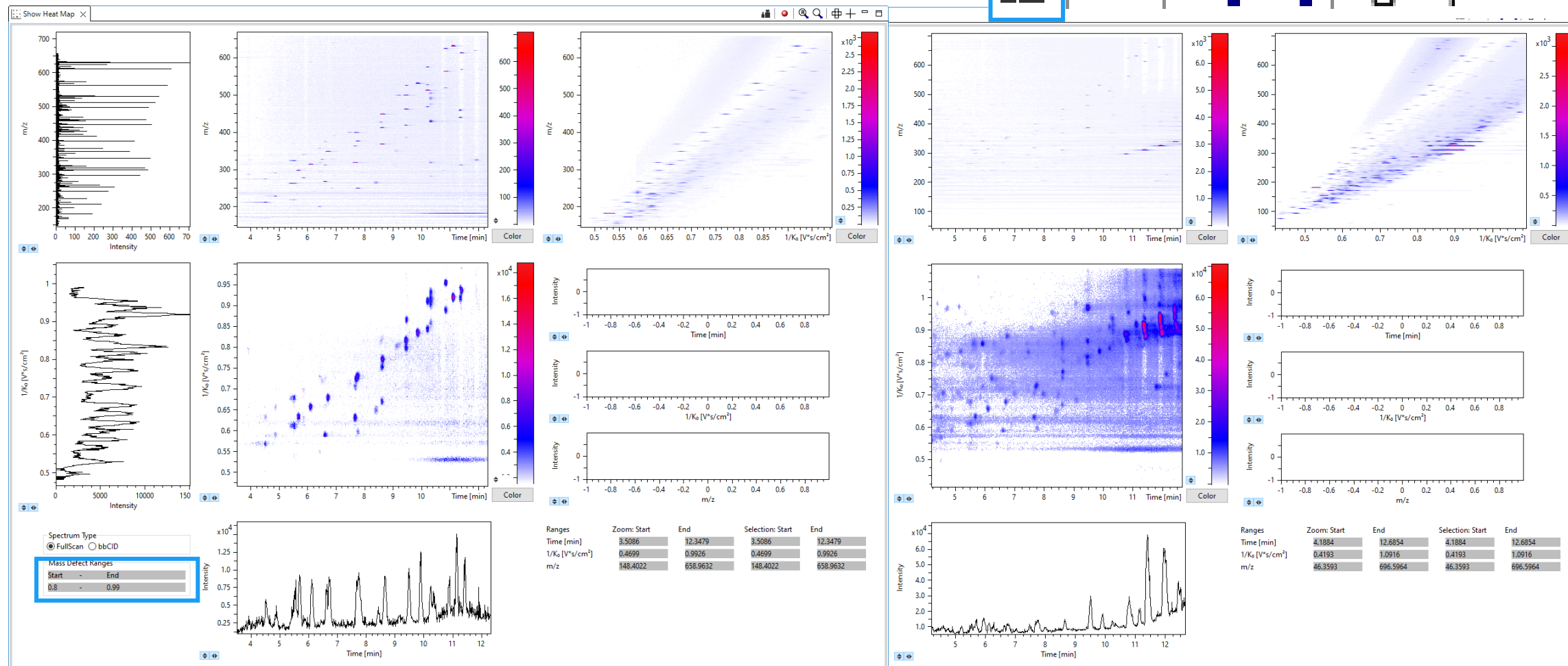
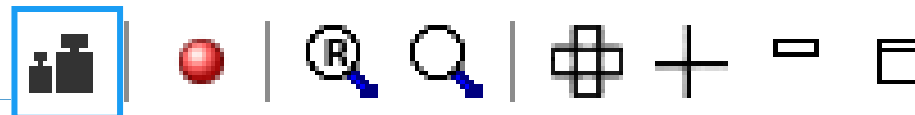
Signal / Noise Parameters	
Algorithm	Smart ▾
S/N filter	3.000
Surrogate noise	1.000
Range left of peak maximum [s]	50.00
Range right of peak maximum [s]	0.00
Points per regression interval	1,000

Signal / Noise Parameters	
Algorithm	Expert ▾
S/N filter	3.000
Surrogate noise	1.000
Range left of peak maximum [s]	50.00
Range right of peak maximum [s]	0.00
Points per regression interval	1,000
Ignore most abundant points [%]	15
Ignore left from peak start by FWHM factor	0.50
Ignore right from peak end by FWHM factor	1.00

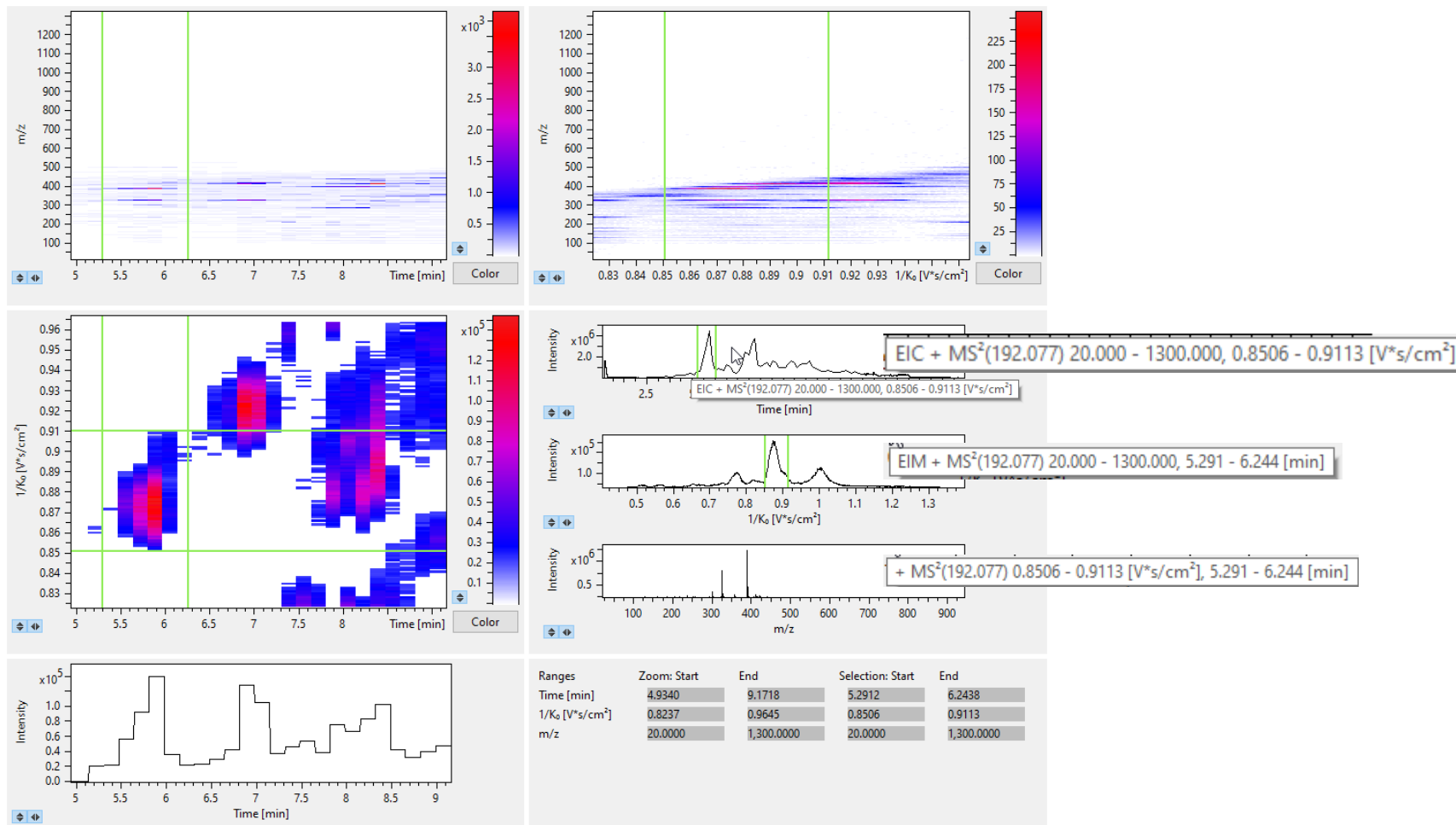
Heat Map View: Switch Spectrum Type



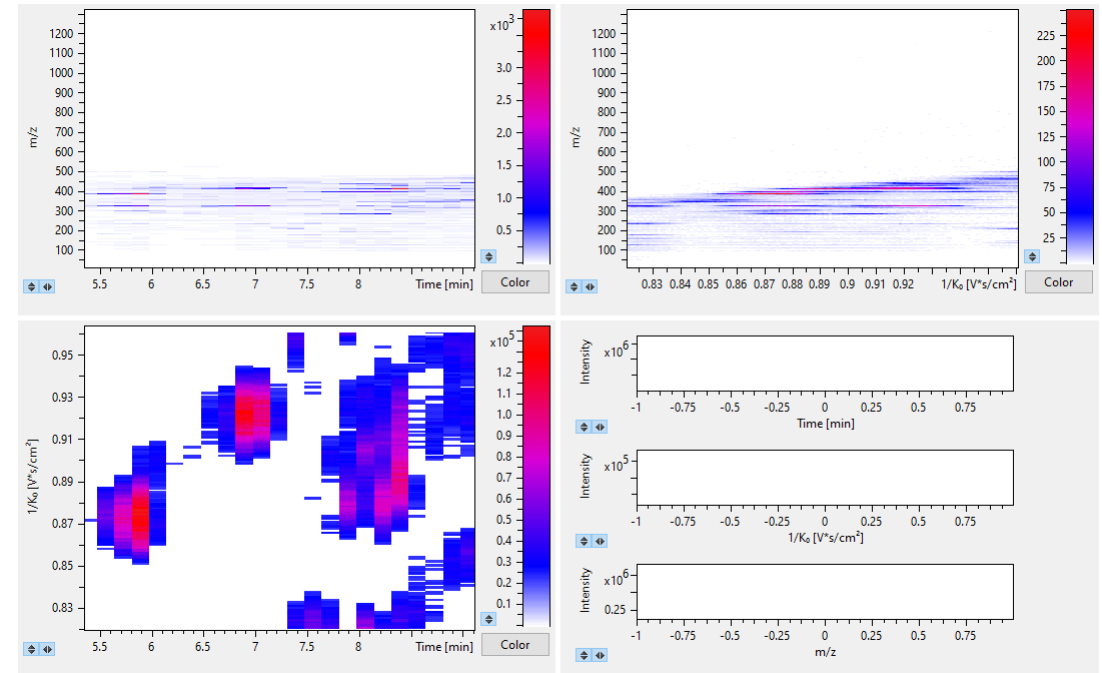
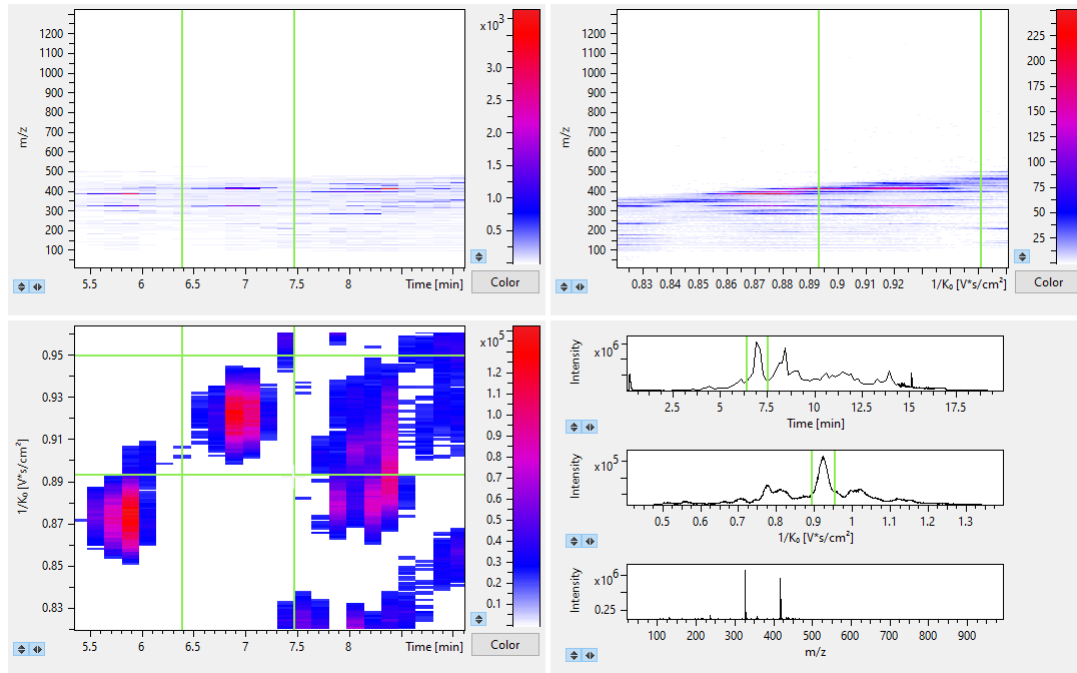
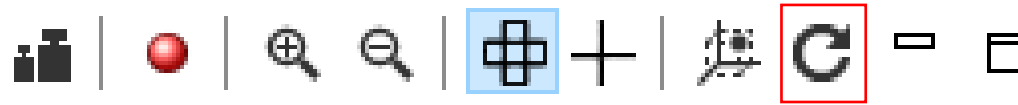
Heat Map View PFAS – Fullscan – Mass Defect Filter 0.8 – 0.99



Improvements HeatMap: Tooltips to Show Filter Ranges



Show HeatMap: Reset Selection Ranges



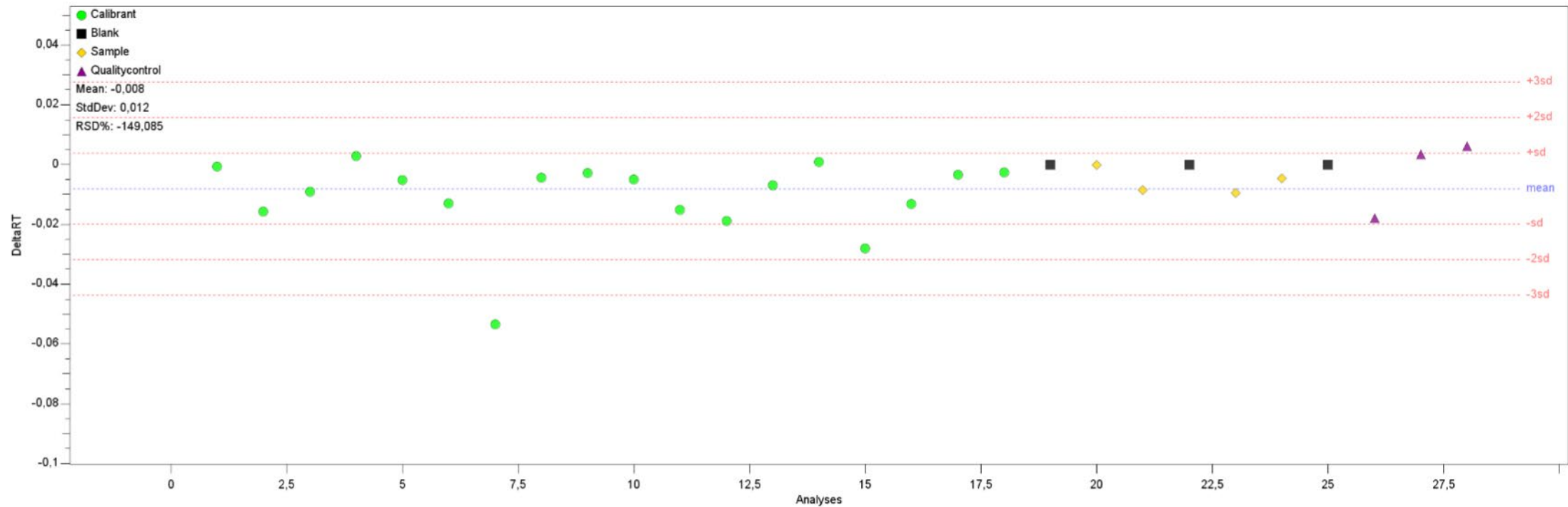
Improvements Show HeatMap: Send Selection Ranges to Show Views

- Add selected ranges to show views for further investigations



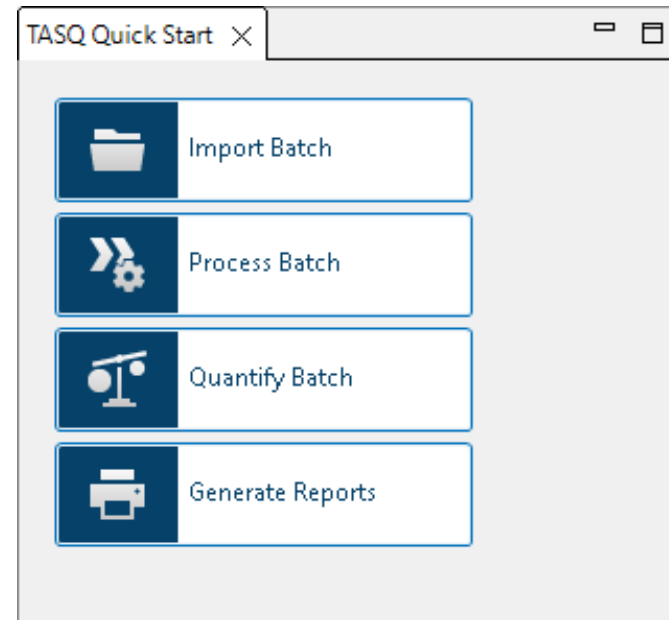
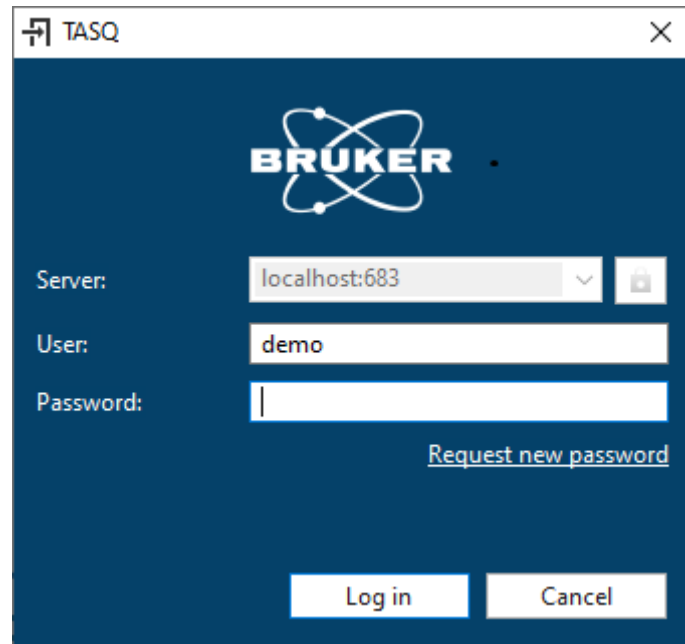
Improvements Report Data Provider

- Batch Statistics Chart Item in development

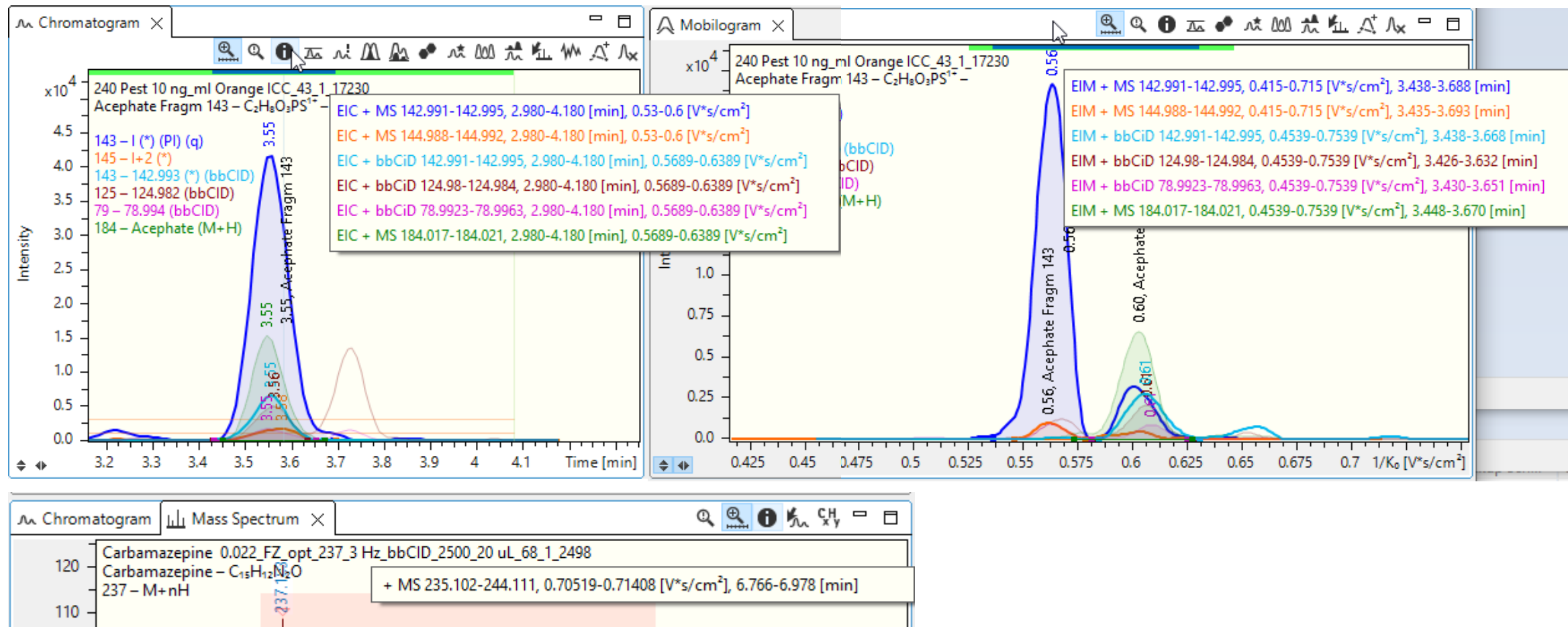


New Corporate Design for Bruker Ribbon Bar

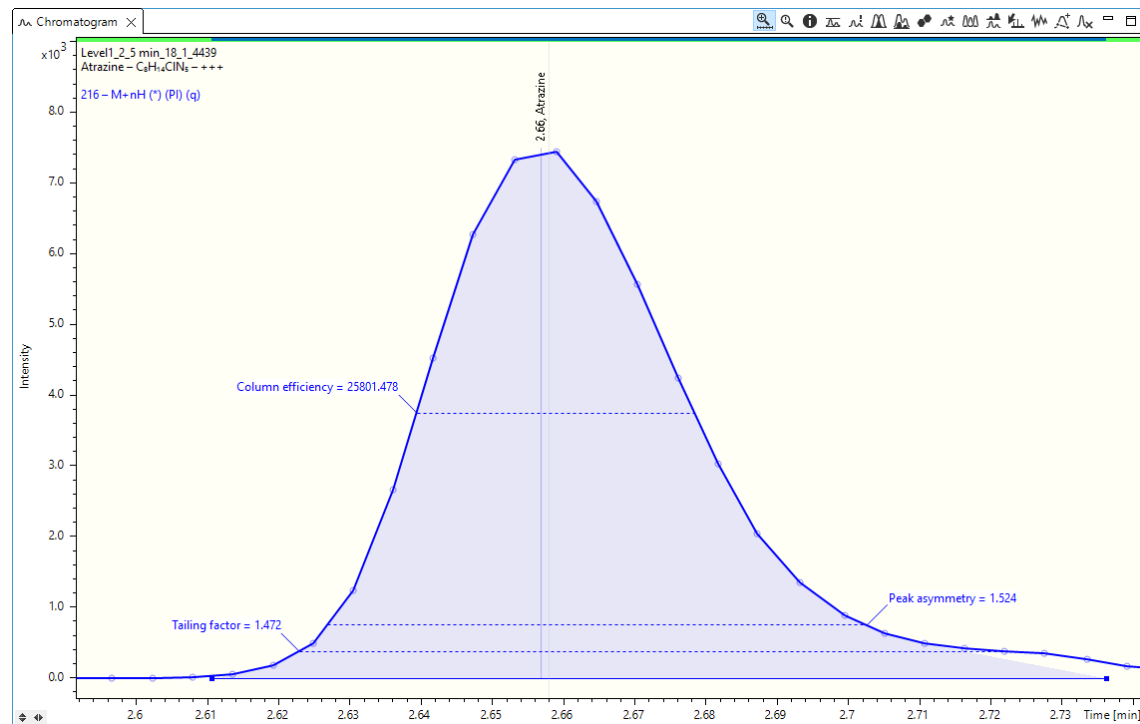
- Our Corporate Designs improves more and more



Detailed Information of how Traces were Constructed



Peak Symmetry Factors in Chromatogram/Mobilogram View only



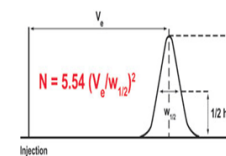
EIC + MS 216.098-216.104, 1.908-3.408 [min], CE 25801.478, PA 1.524, TF 1.472

- <https://www.silicycle.com/faq/hplc/how-are-column-efficiency-peak-asymmetry-factor-tailing-factor-and-resolution-calculated>

Column efficiency calculation

Column efficiency, indicated as the number of theoretical plates per column, is calculated as $N = 5.54 (t_R / W_{0.5})^2$ where t_R is the retention time of the analyte of interest and $W_{0.5}$ the width of the peak at half height.

This half-height method enables the determination of the number of theoretical plates per column (N) even if the peak is not fully separated from a neighbouring peak (poor resolution), as long as the valley between the peaks is lower than the half-height of the peak. Half-height measurements commonly is the method of choice for automatic determination by data systems.

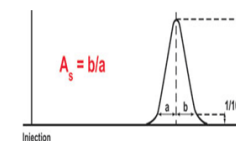


The larger the number of theoretical plates per column, the sharper the peak! Should you need to calculate the number of theoretical plates per meter, you must use the following equation:

$$\text{Number of theoretical plates per column} \times 100 / \text{length of HPLC column (cm)} = \text{Number of theoretical Plates per m}$$

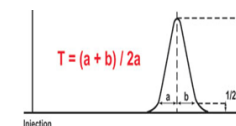
Peak Asymmetry Factor

Peak Asymmetry Factor, often presented as A_s , is calculated with the following equation $A_s = b/a$ where b is the distance from the peak midpoint (perpendicular from the peak highest point) to the trailing edge of the peak measured at 10% of peak height and a is the distance from the leading edge of the peak to the peak midpoint (perpendicular from the peak highest point) measured at 10% of peak height. If $A_s > 1$: tailing, et si $A_s < 1$: fronting



Tailing Factor

Tailing Factor (T_f) is the USP coefficient of the peak symmetry. It is calculated using the following equation: $T_f = (a+b)/2a$ where a is the distance from the leading edge of the peak to the peak midpoint (perpendicular from the peak highest point) measured at 5% of peak height and b is the distance from the peak midpoint (perpendicular from the peak highest point) to the trailing edge of the peak measured at 5% of peak height.



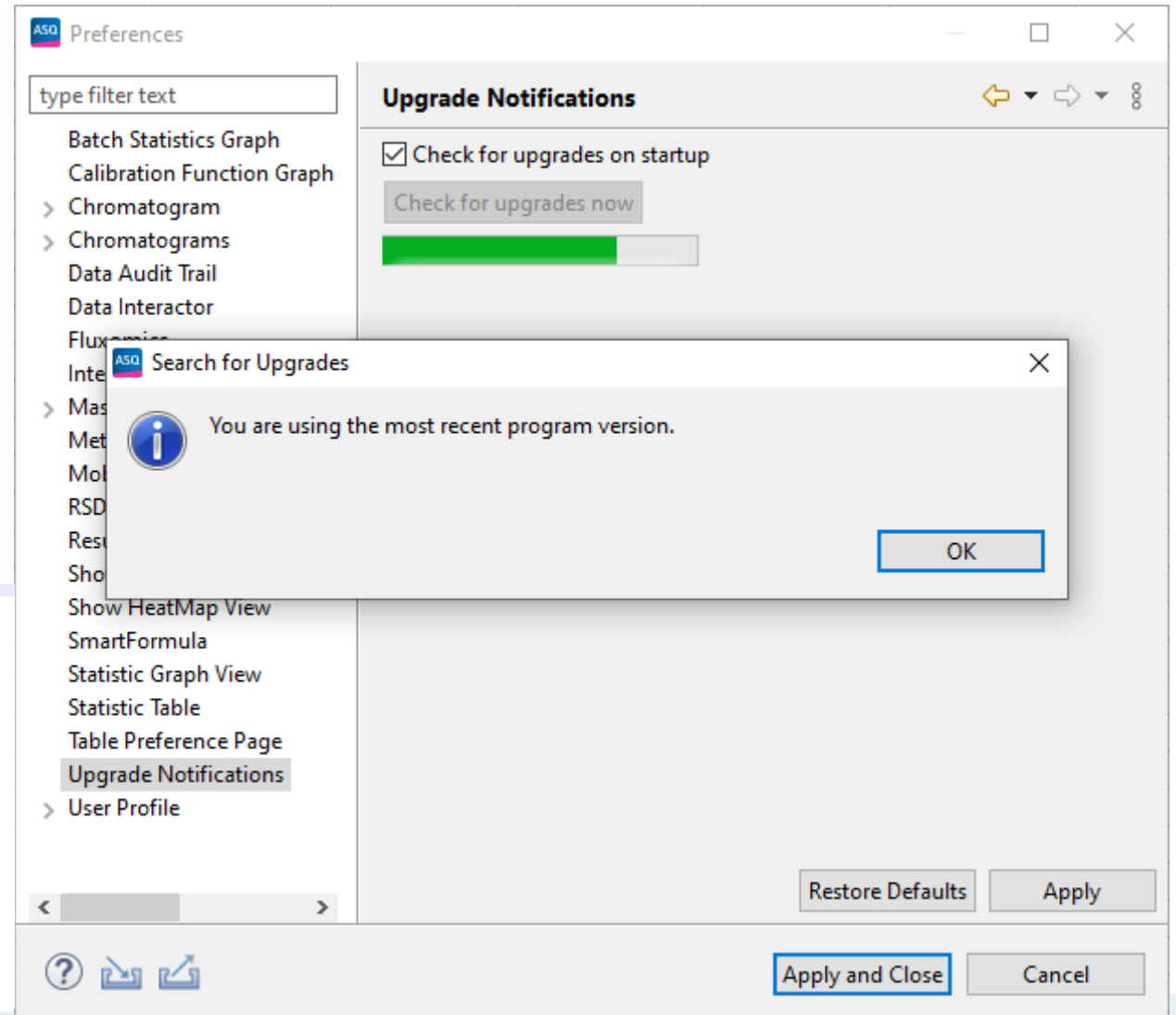
Show Notification that a Newer SW Version is Available for Download

- Check for new versions each time TASQ client is started
- Or check explicitly whether a new version is available from Preferences>>Upgrade Notifications pane

```

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8         <description> Most recent changes of MetaboScape</description>
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27        <description>something French</description>
28      </language>
29    </languages>
30  </download>
31 </downloads>
32

```



The screenshot shows the 'ASQ Preferences' dialog box. On the left is a tree view with 'Upgrade Notifications' selected. The right pane shows the 'Upgrade Notifications' settings, including a checked checkbox for 'Check for upgrades on startup' and a 'Check for upgrades now' button. A modal dialog box titled 'ASQ Search for Upgrades' is open in the foreground, displaying an information icon and the text 'You are using the most recent program version.' with an 'OK' button.

Show Notification that a Newer SW Version is Available for Download

The dialog box titled "ASQ Upgrade Notification" displays "New Upgrades available". It lists two upgrade options:

- TASQ 2023a**: Most recent changes of TASQ. Includes a [Download](#) link.
- TASQ 2023b**: Most recent changes of TASQ. Includes a [Download](#) link.

At the bottom, there is a checkbox labeled "Do not notify me again for above versions" which is currently unchecked. "OK" and "Cancel" buttons are at the bottom right.

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32
```

The "ASQ Preferences" dialog box shows the "Upgrade Notifications" section. The "Check for upgrades on startup" checkbox is checked. A "Check for upgrades now" button is present. A green progress bar is visible below the checkbox.

Overlaid on this is a smaller dialog box titled "ASQ Search for Upgrades" with an information icon and the message: "You are using the most recent program version." with an "OK" button.

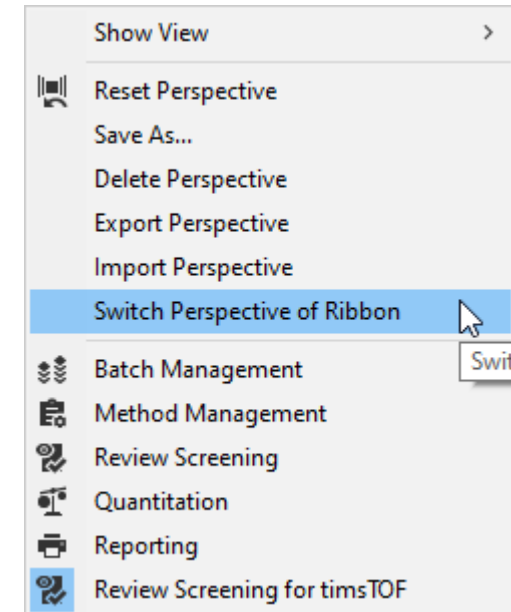
At the bottom of the Preferences dialog are "Restore Defaults", "Apply", "Apply and Close", and "Cancel" buttons.

Improved Handling of Perspectives

Export / Import of perspectives enabled

- User can save a perspective as brxpr file
 - To save it to restore it later
 - To share with peers
 - To transfer it to another client system

The Bruker ribbon buttons can be assigned to show other stored perspectives



Change the Default Perspective for Bruker Ribbon Buttons

ASQ Switch default ribbon perspective

Available ribbons of application to switch default perspective
Select the desired ribbon by right-clicking with the mouse

- Batch Management
- Method Management
- Review Screening
- Quantitation
- Reporting

Buttons: ? < Back Next > Finish Cancel

ASQ Switch default ribbon perspective

List of perspectives for the selected ribbon
Select the new default perspective by double-clicking with the mouse

Default	Name of perspective	Type of perspective
	Review Screening	System perspective
<input checked="" type="checkbox"/>	Review Screening for timsTOF	User defined perspective

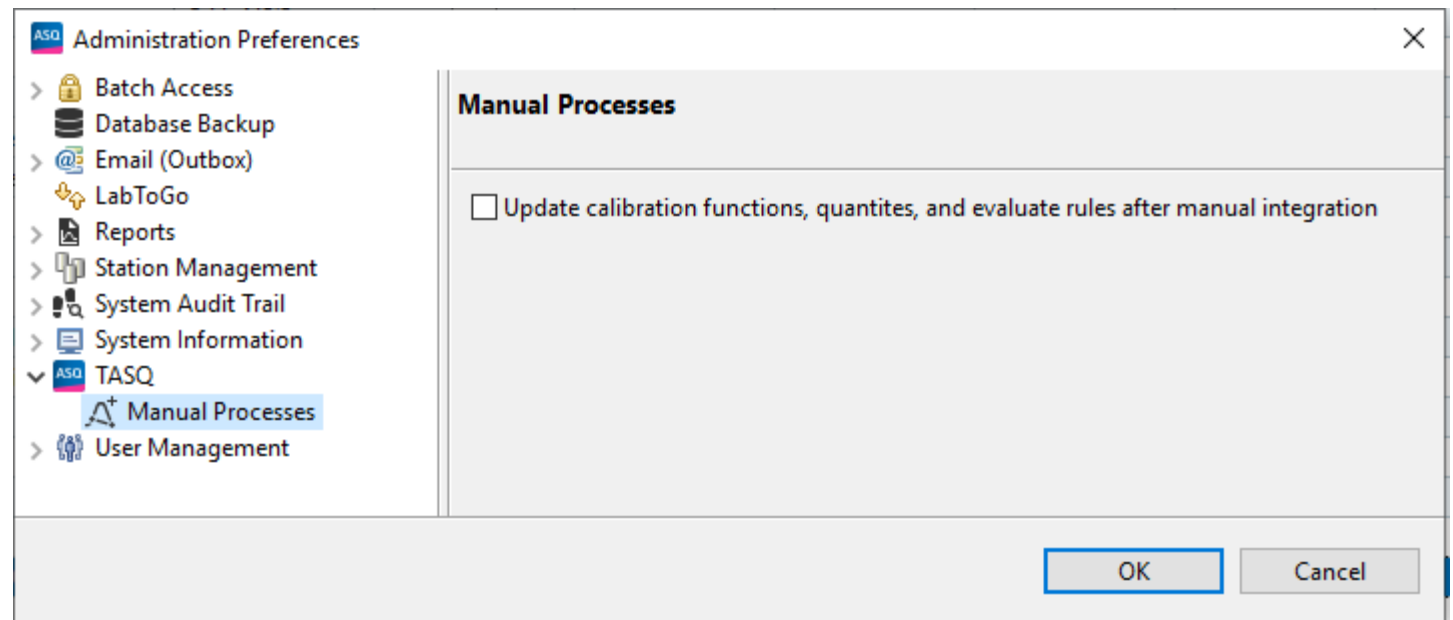
Buttons: ? < Back Next > Finish Cancel

Performance Manual Integration: Optionally Switch Off Downstream Processes

- TASQ <= 2023A handles internal standards with multiple chromatographic peaks poorly
 - In TASQ <= 2023A only the signal of one ion is used (principle ion)
 - → Change to use the summed intensity of all quantifier ions
- Each time a manual integration of a calibration sample is performed TASQ automatically updates many other determinations in order to keep all quantity values up to date
 - → For TASQ 2023 A SR1 add an option in bdal.properties to switch off the downstream process
 - → For TASQ 2023 B offer an option that user can specify the behavior (perform downstream process: yes|no) in the GUI
 - → Invalidate quantity values as used
 - → User starts quantification of batch as soon as all manual corrections have been done

Performance Manual Integration: Optionally Switch Off Downstream Processes

- Create a TASQ 2023A SR1 with quick fixes in tasq server only
- Offer option in TASQ 2023B in GUI
- Information is persisted in Compass DB
- Option is applied globally to all users



Miscellaneous

- Ongoing work on Audit trail
 - Closing more gaps
 - Integrating improvements from compass platform
- Rename intensity threshold to height threshold -> behavior of peak detection of chromatograms and mobilograms changed: peaks are discarded if their peak height is lower than the threshold. This avoids false positives as intensity on noisy data is not a suitable criterion
- Import multiple tasqMethod files at once

Miscellaneous

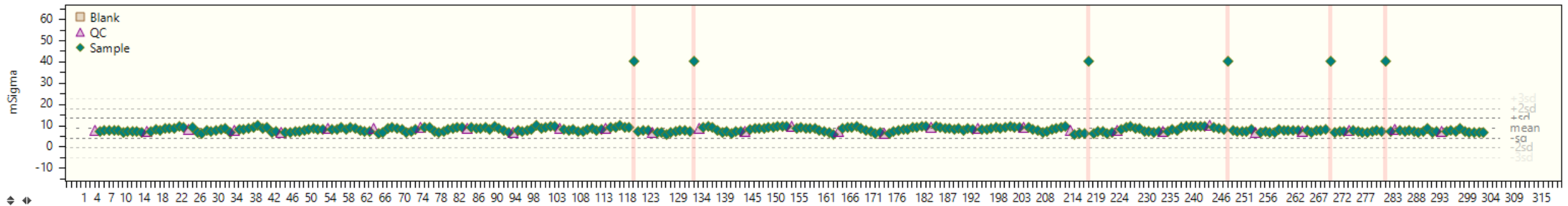
- Keep zoom ranges on selection changes in mobilogram and chromatogram view
 - on selection changes
 - or manual integration
- Show same traces after manual integration as before, do not switch to show all traces of determination
- Option to show mobilogram of internal standard in mobilogram view added
- Show only traces of mandatory ions for reference data sets if this option is activated in views
- Option to show QC in calibration function graph added
- For calculating signal of internal standards for quantiation use information of all specified quantifier ions

Miscellaneous

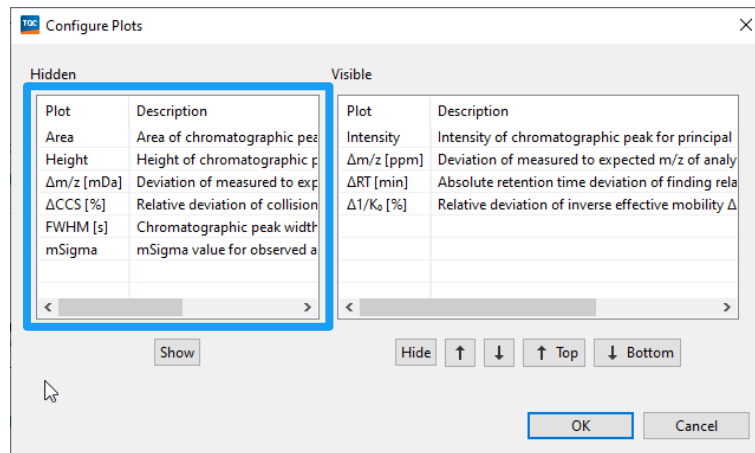
- Delete analytes in analyte settings table of method editor using DEL key
- Improving selection of items in wizards: allow multiselection – toggle state selected yes : no
- When changing filter for method selection in processing wizard apply the new filter settings to method navigator as well
- General improvements on name checking when saving methods or other data, added error decorators
- Renovation of wizards – migrate from old nat tables to new nat tables
 - Batch Parameter Wizard
 - Batch Concentration / Levels
 - Batch Processing/Reprocessing wizards
 - Configure Ion – Peak Ranges wizard

New in TASQ RealTimeQC

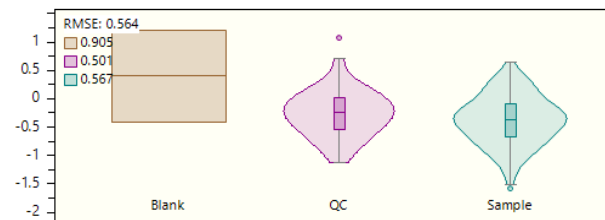
New outlier detection logic (sample type specificity, 1sd/2sd/3sd)



New plot types

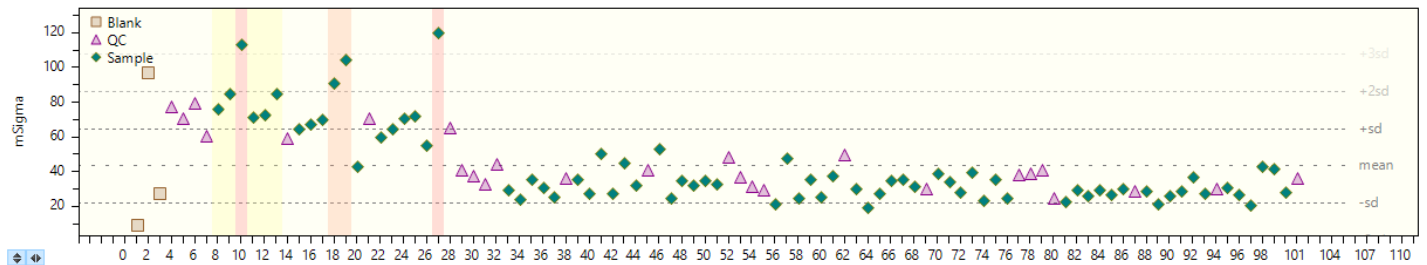
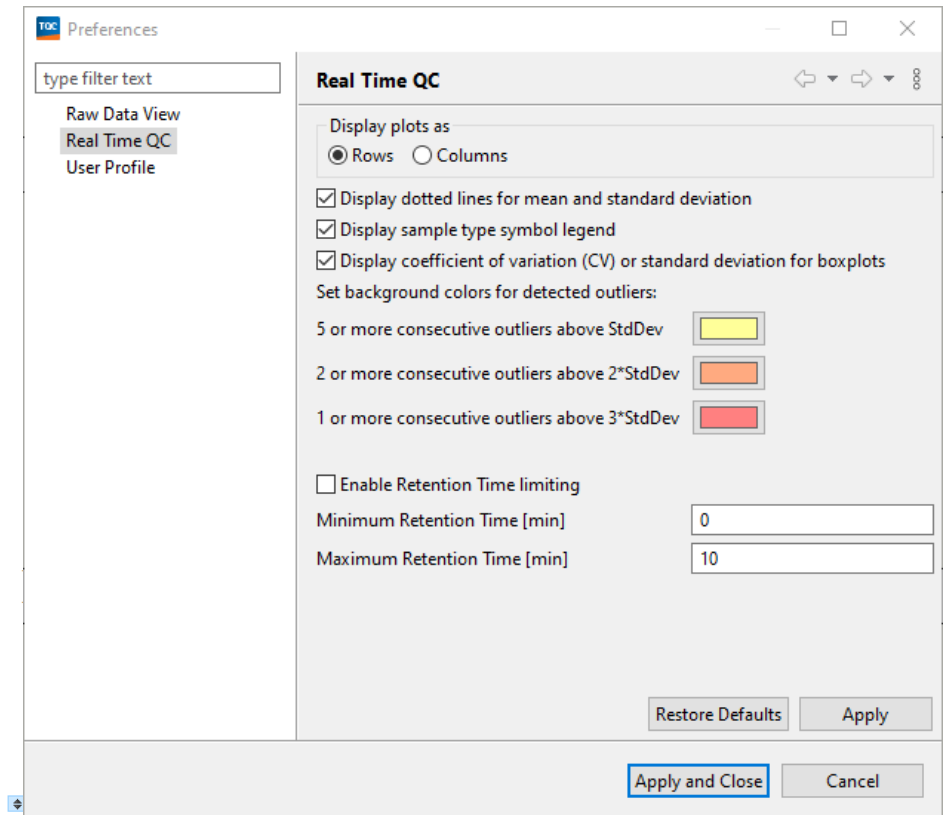


Sample types shown in violin plot RMSE calculation for $\Delta m/z$ ppm



New in TASQ RealTimeQC

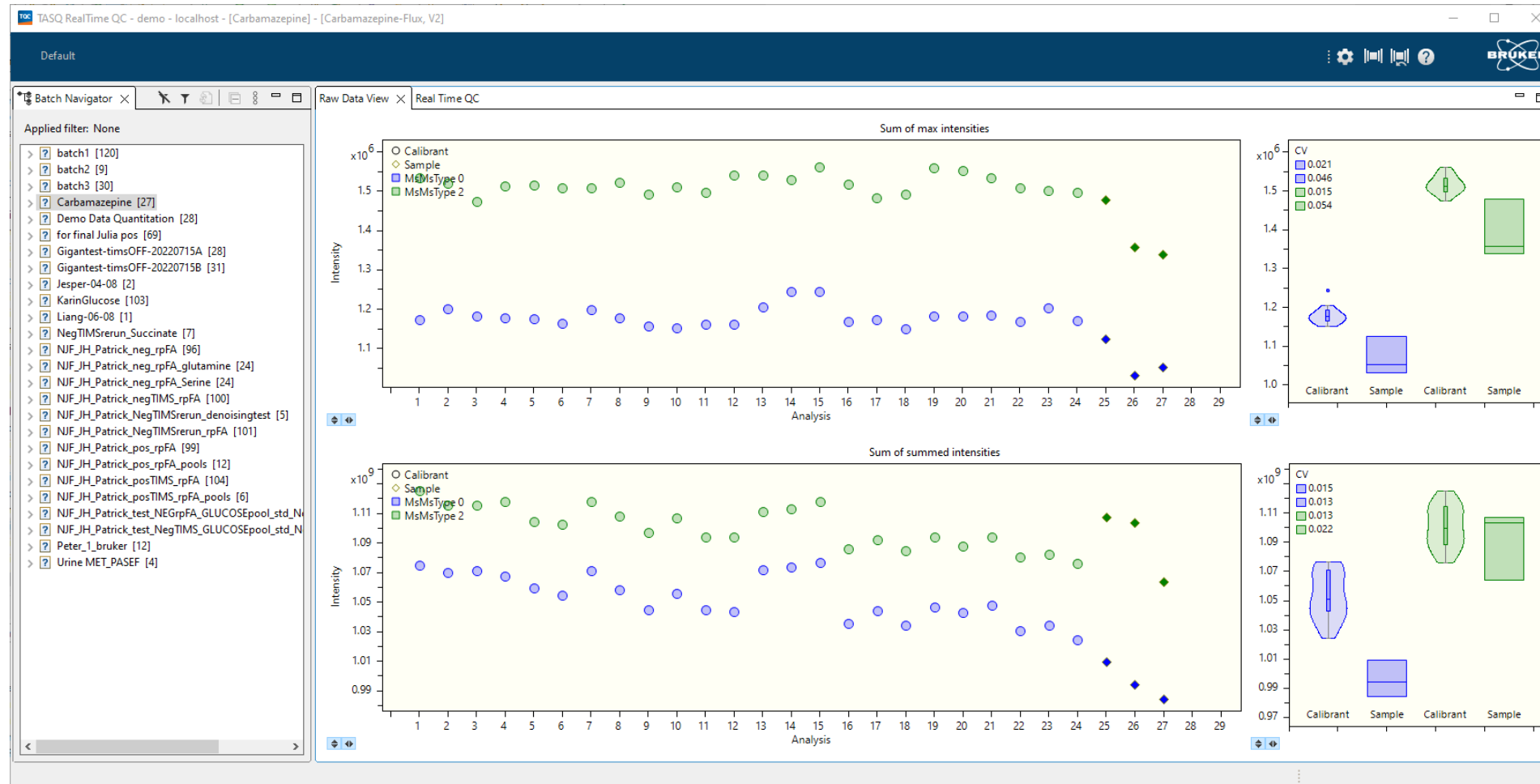
- Different rules for outlier
 - Outlier > 3 sd
 - 2 consecutive outliers > 2 sd
 - 5 consecutive outliers > 1 sd,...

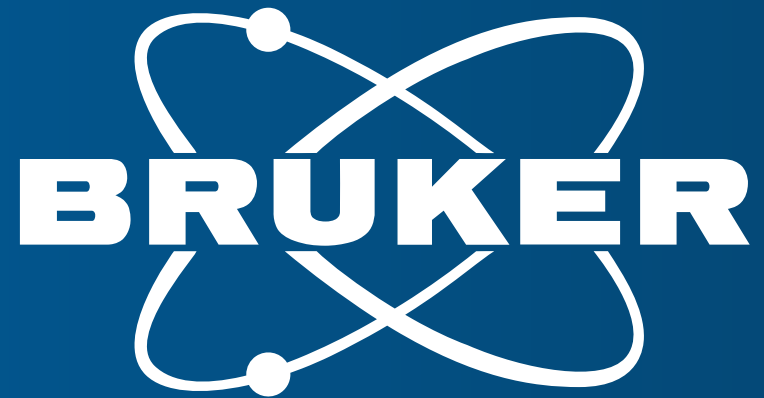
The screenshot shows the 'Preferences' dialog box with the 'Real Time QC' tab selected. The settings are as follows:

- type filter text
- Raw Data View
- Real Time QC**
- User Profile
- Display plots as: Rows Columns
- Display dotted lines for mean and standard deviation
- Display sample type symbol legend
- Display coefficient of variation (CV) or standard deviation for boxplots
- Set background colors for detected outliers:
 - 5 or more consecutive outliers above StdDev:
 - 2 or more consecutive outliers above 2*StdDev:
 - 1 or more consecutive outliers above 3*StdDev:
- Enable Retention Time limiting
- Minimum Retention Time [min]:
- Maximum Retention Time [min]:
- Buttons: Restore Defaults, Apply, Apply and Close, Cancel

TASQ RealTime QC Statistics Based on Raw Data – TIC – Max Int



- Add Σ TIC overview to TASQ RealTimeQC retrieved from directly from raw data



Innovation with Integrity