TASQ 2023

What’s New

WHAT'S NEW

01 Main Features

02 Minor Features

03 Obstacles

Main Features

- Adapt to new Corporate Design – new program icon ASQ – new icons in TASQ client
- Enable multiple mobility values $1/K_0$ per analyte – support of adducts, protomers, fragment ions generated in the ion source
- CCS quality information – add information of quality / source of CCS value
- Show Heat Map View – enable deep insight into timsTOF data
- Fit exponentially modified peaks into detected chromatographic / mobilogram peaks
- TASQ RealTime QC Monitor Tool

Minor Features

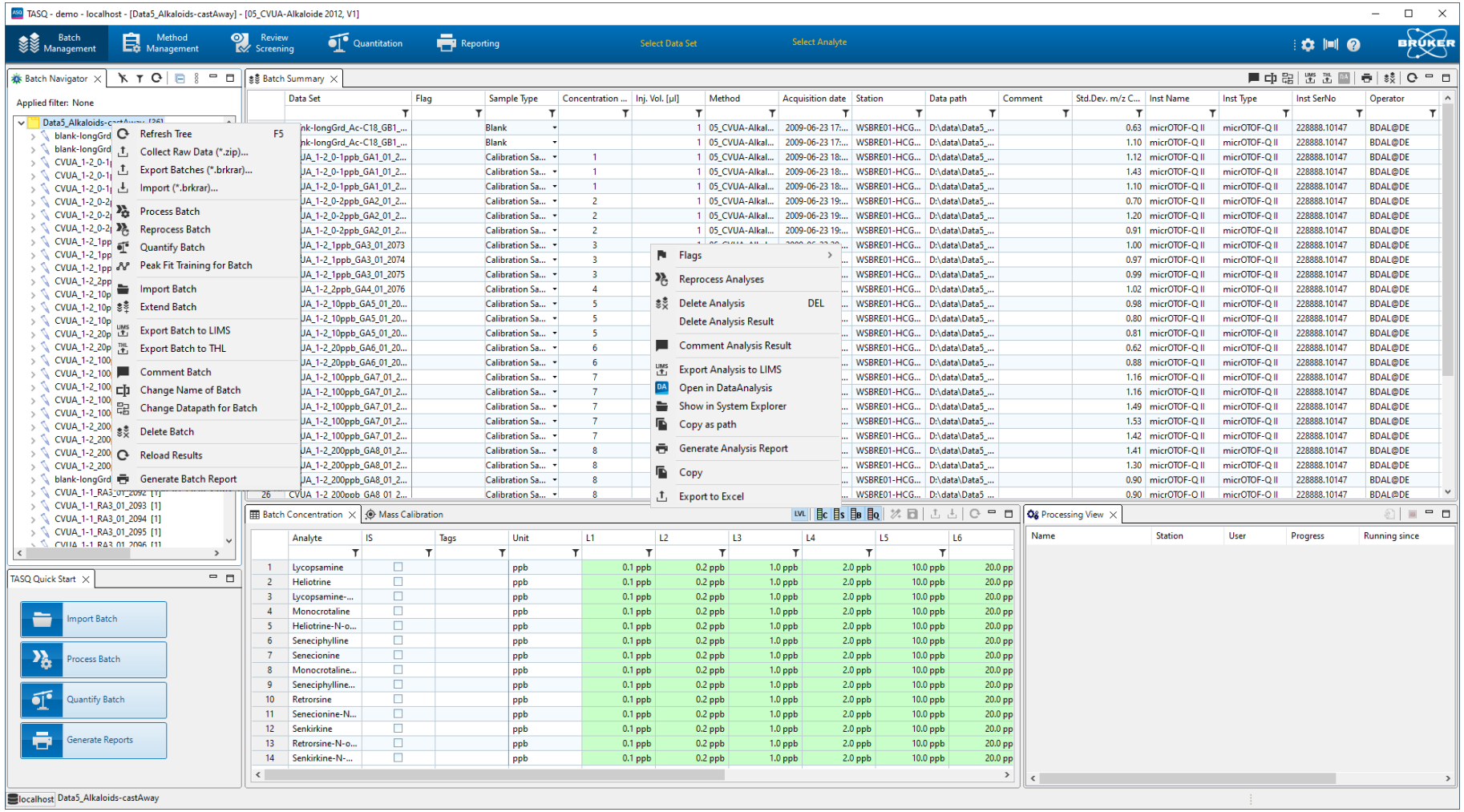
- Base peak chromatograms (BPCs) generated for timsTOF data
- BPCs are shown in correct order in chromatogram view
- Changed behavior of peak detection algorithm: instead of intensity threshold a height threshold will be used to test the detected peak based on peak height and not by peak intensity
- Improved labels in Show Chromatogram, Mobilogram, MS Spectrum views
- Multi-selection of ions in Detailed Analyte Ion Results view enabled – selected ion's traces will be shown
- Analyte's tag column in Batch Concentration View added
- Save as timsTOF method dialog suggest a method name
- Imported batch is selected in batch navigator automatically
- Imported method is selected in method navigator automatically
- Smart Formula view shows selected *m/z* value

Minor Features

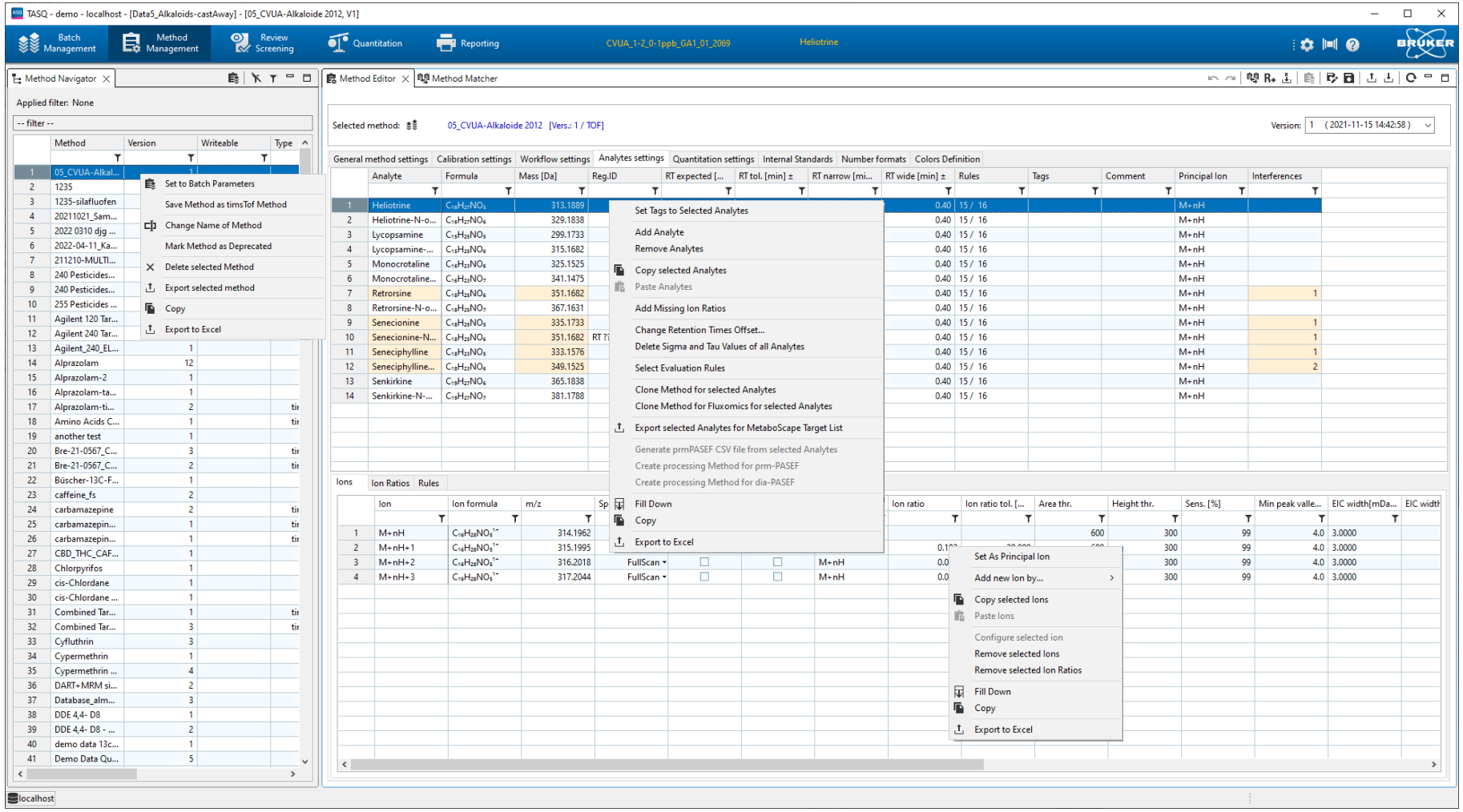
- Show notifications if disk is running full
- Multi-selection for tables in wizards enabled
- Creation of prmSettings.sqlite files discontinued
- Denoising of timsTOF data is not supported
- Heap size for TASQ client increased to 2048M
- Improved performance of large result tables

New Corporate Design – Program Icon and Splash Screen

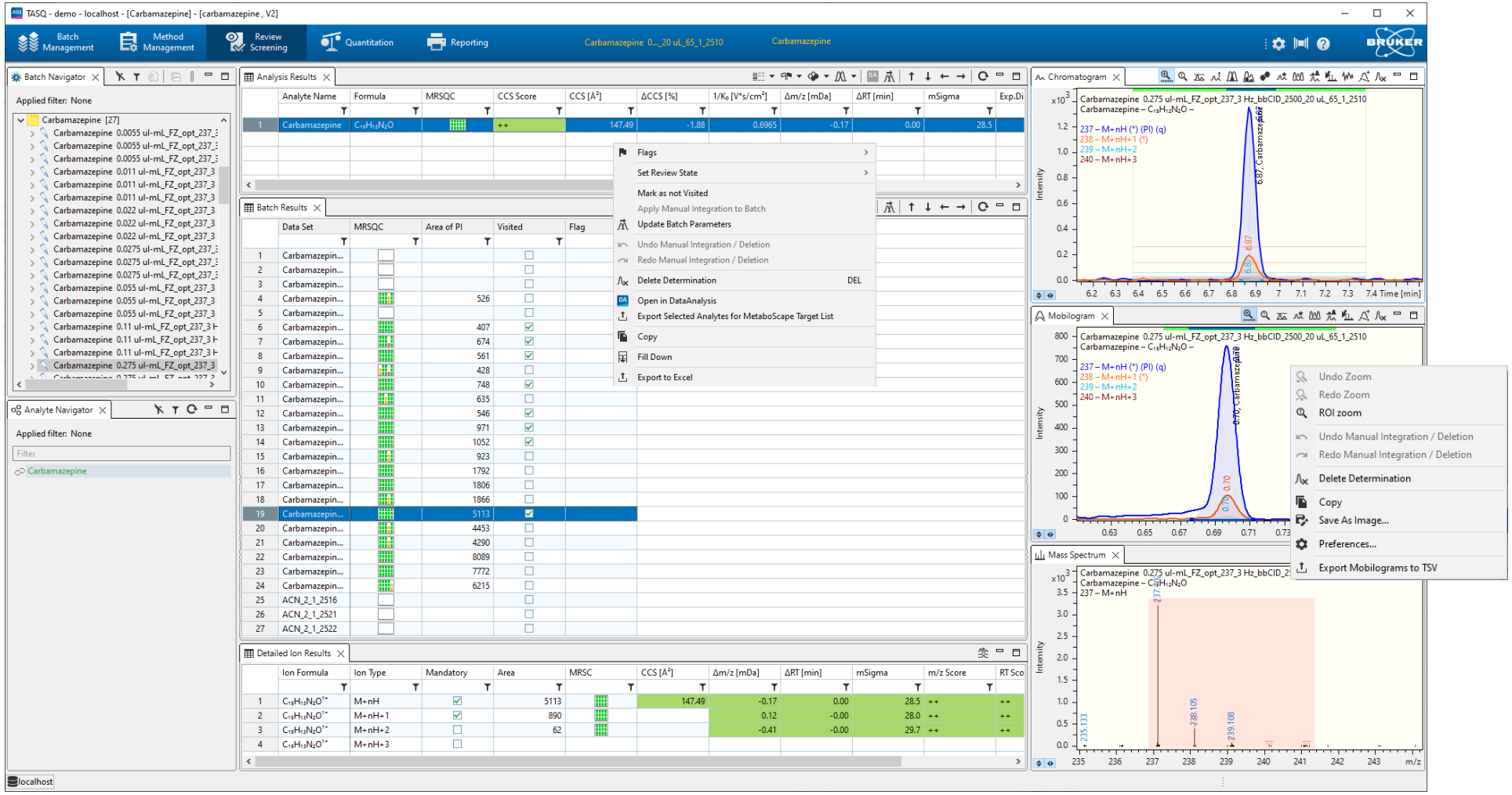
New Corporate Design – Icons – Batch Management Perspective



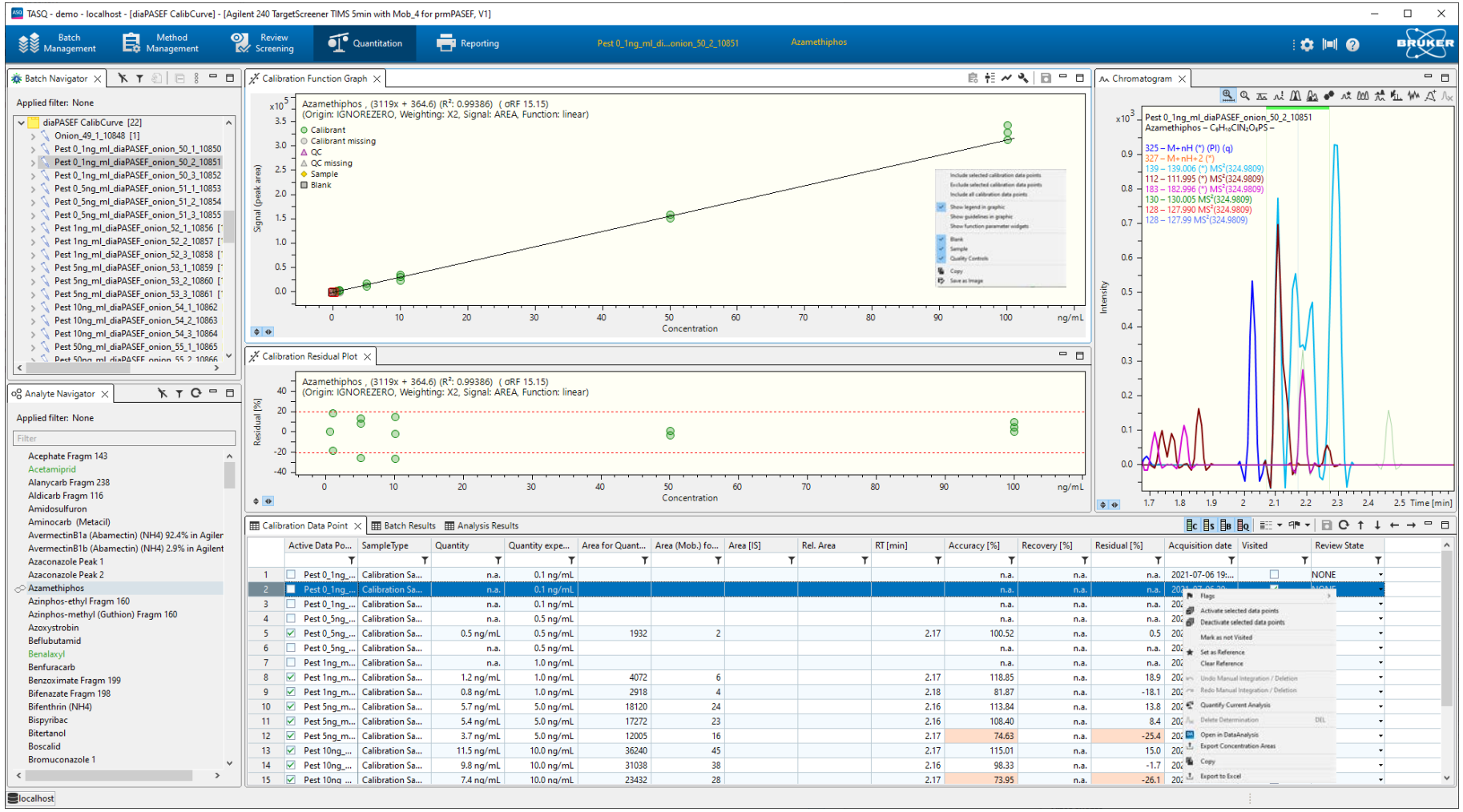
New Corporate Design – Icons – Method Management Perspective



New Corporate Design – Icons – Result Review Perspective



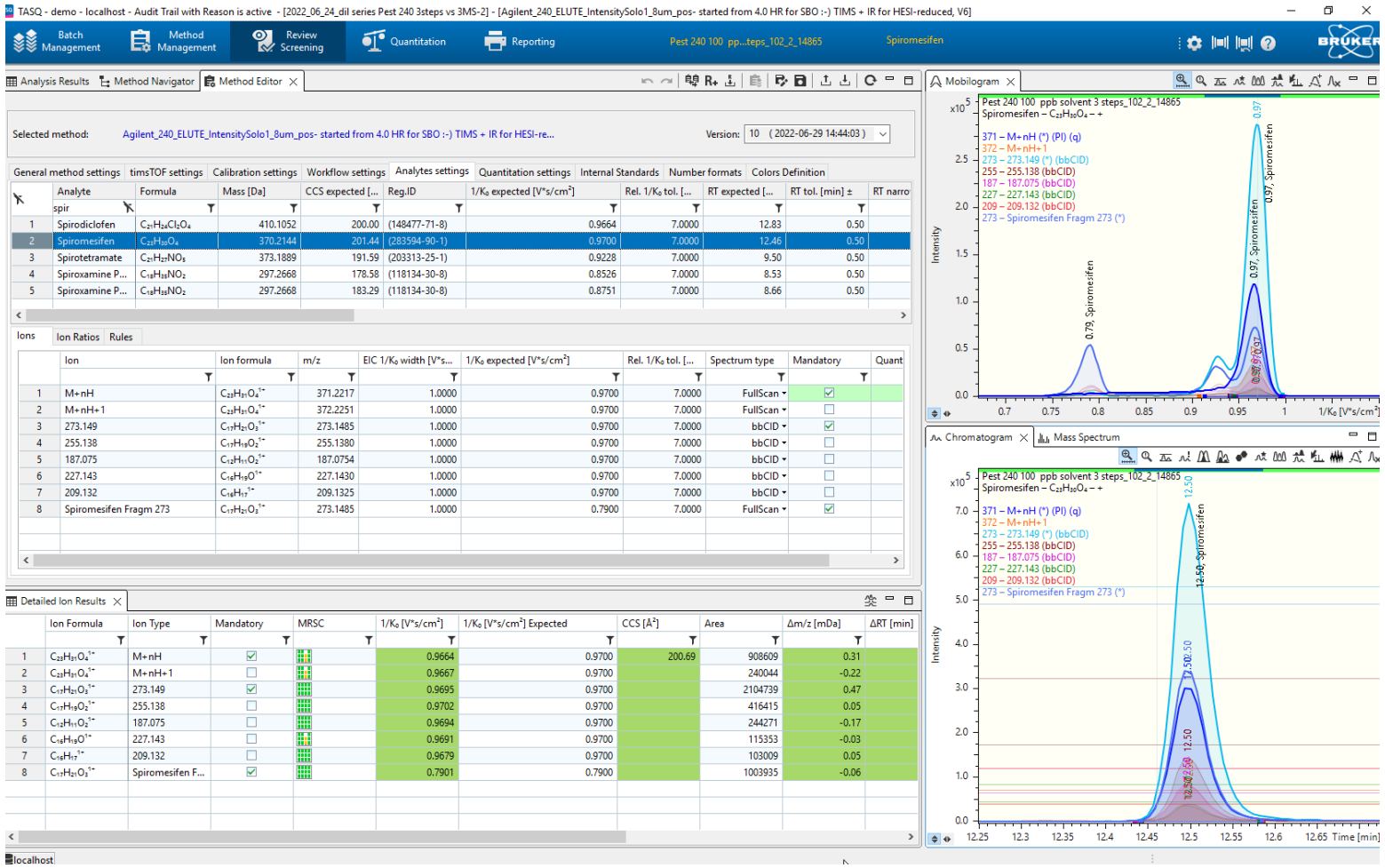
New Corporate Design – Icons – Quantitation Perspective



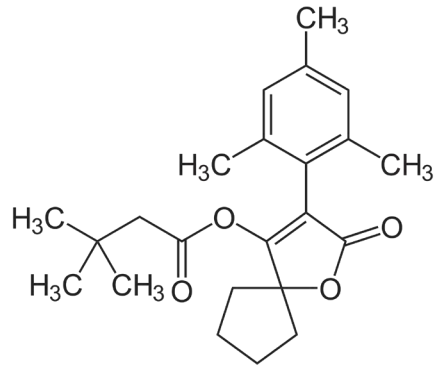
Enable multiple mobility values $1/K_0$ per analyte

- Individual $1/K_0$ values can be specified for each ion in the ion parameter settings table in method editor
- If no mobility information is given for an ion the analyte's mobility information is used for processing
- Additionally, a relative $1/K_0$ threshold can be specified for each ion individually
- These values can be specified in a csv file which will be imported by Create Method…
- Determinations are built by collecting ions with chromatographic peaks with the same retention time and peaks with matching $1/K_0$ values specified in the method
- Copy and paste of ions within an analyte in ions editor enabled

Enable multiple mobility values $1/K_0$ per analyte

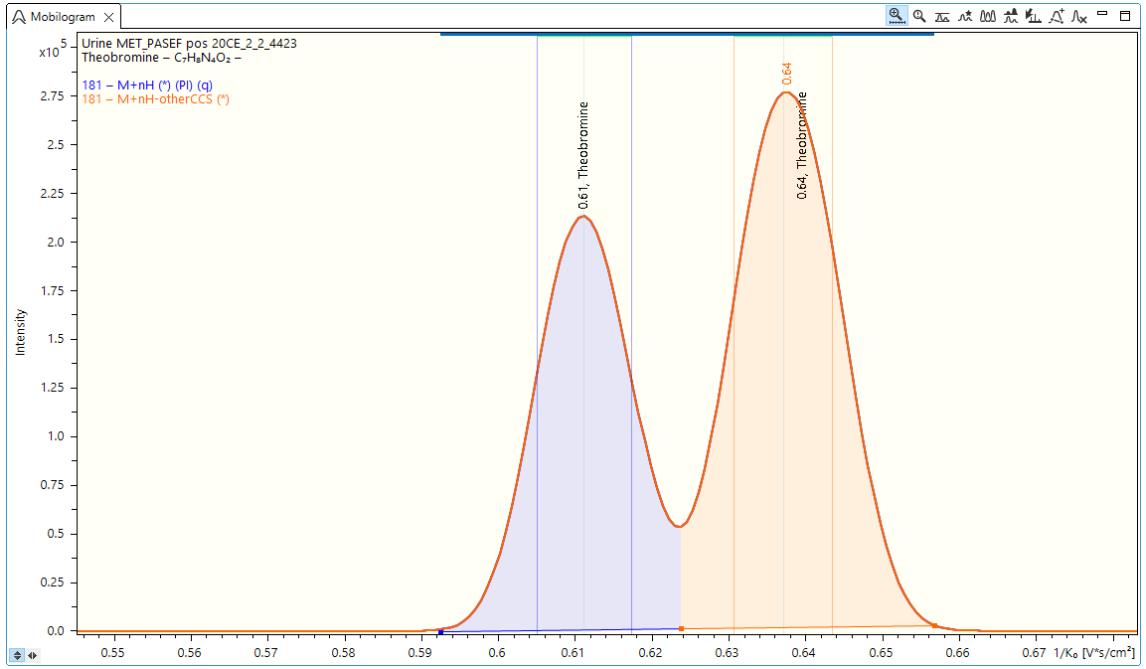


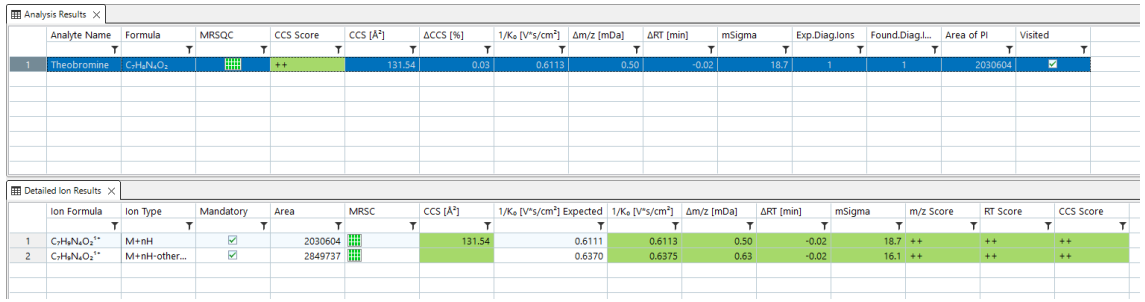
- Spiromesifen

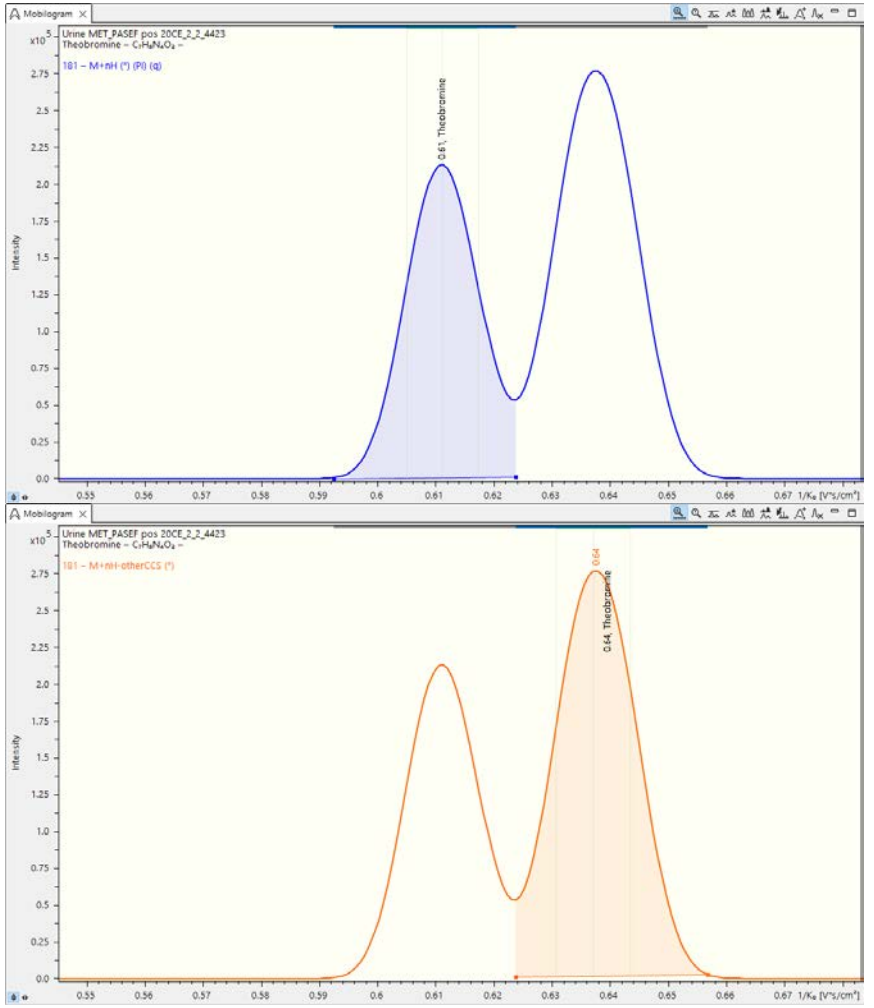


- Small peak at $1/K_0$ 0.79 Vs/cm²
- Major peak at $1/K_0$ 0.97 Vs/cm²

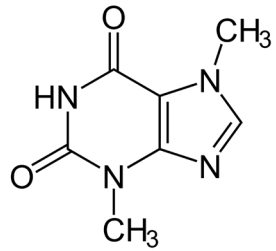
Enable multiple mobility values $1/K_0$ per analyte







- Theobromine
- Mutiple $1/K_0$
- 0.61 Vs/cm^2
- 0.69 Vs/cm^2



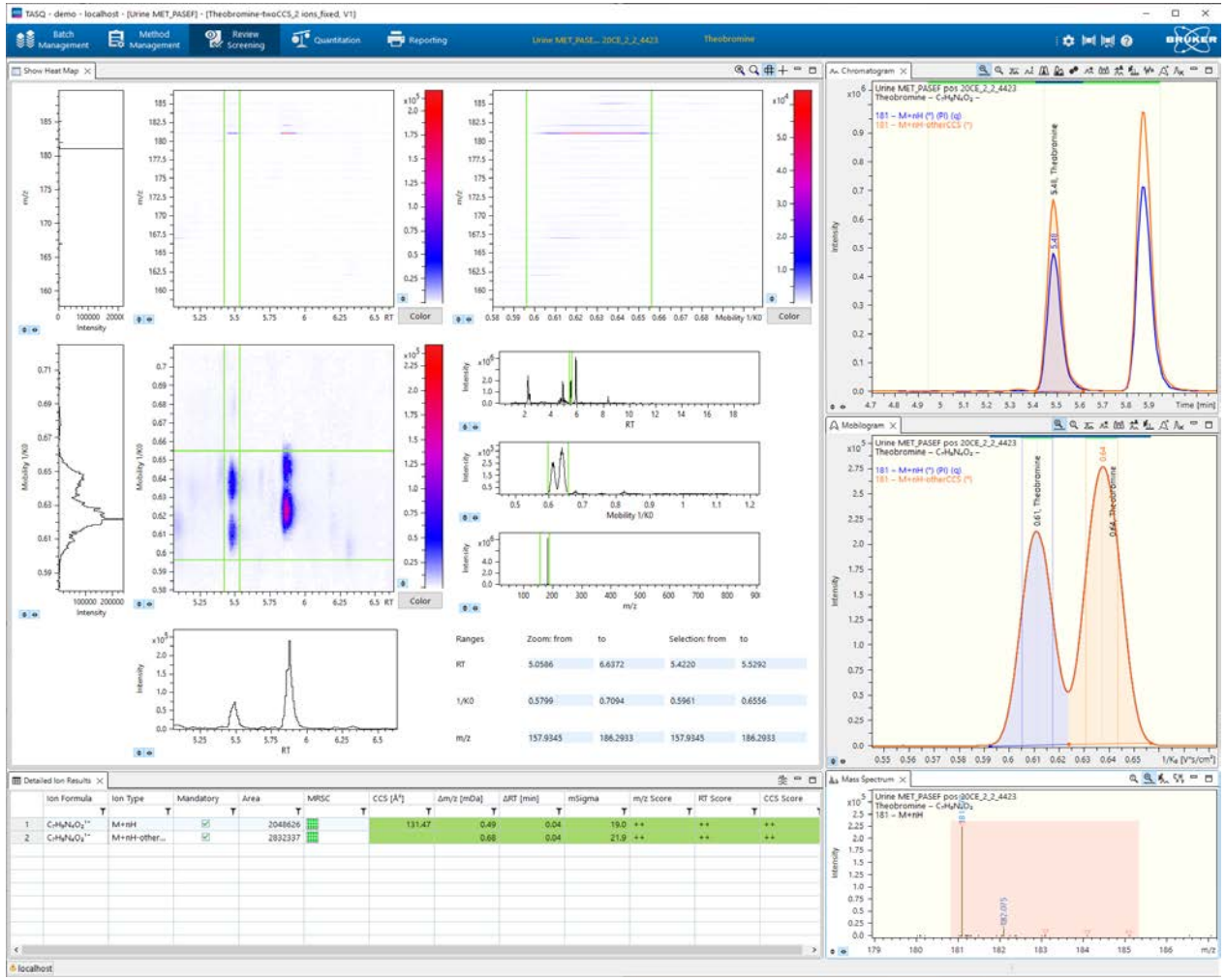
CCS Quality Information

- Additional information about the quality and origin of the mobility information can be specified in the tasqMethod for each analyte.
- This information can be entered in a csv file which will be evaluated by Create Method… command.
- The information is stored in two parts – CCS Quality Tag and CCS Quality Description.
- CCS Quality Tag can be one of: measured, predicted, literature, unspecified.
- CCS Quality Description is a free text and can be used to add information of a literature citation or a used measurement technique or a specific prediction algorithm.
- The CCS Quality infomation can be shown in the result tables with the processing results.

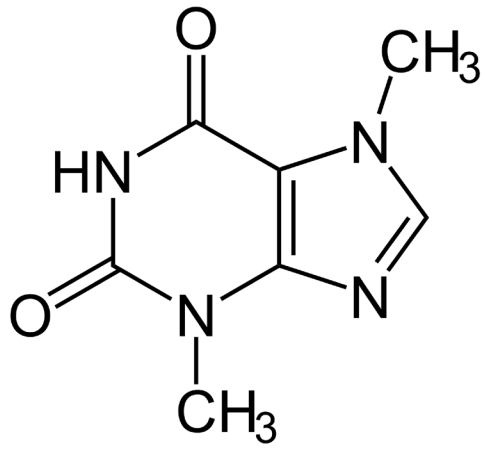
Show Heat Map View – enable deeper insight into timsTOF data

- Show Heat Map view does currently only show data for timsTOF data
- Show Heat Map view shows 2D projections of all three faces of the cube span by Time, Mobility and m/z axis
- For each axis the respective 1D projection is shown
- For each data point in the 2D projections the intensity is coded by color
- The projections are calculated for the currently specified zoom ranges
- The user can zoom in any of the three heat maps to calculate new projections on smaller ranges
- The projections are calculated considering information of each data point within the zoom ranges
- The user can select ranges in the heat maps and TASQ calculates extracted ion chromatograms (EIC), extracted ion mobilograms (EIM) and average MS spectrum using the intervals selected by the range selection mode tool. The calculated traces are shown in the lower right pane of the Show Heat Map view.
- Determinations can be overlayed to the heat maps and the user can select a determination / ion with the determination selection tool

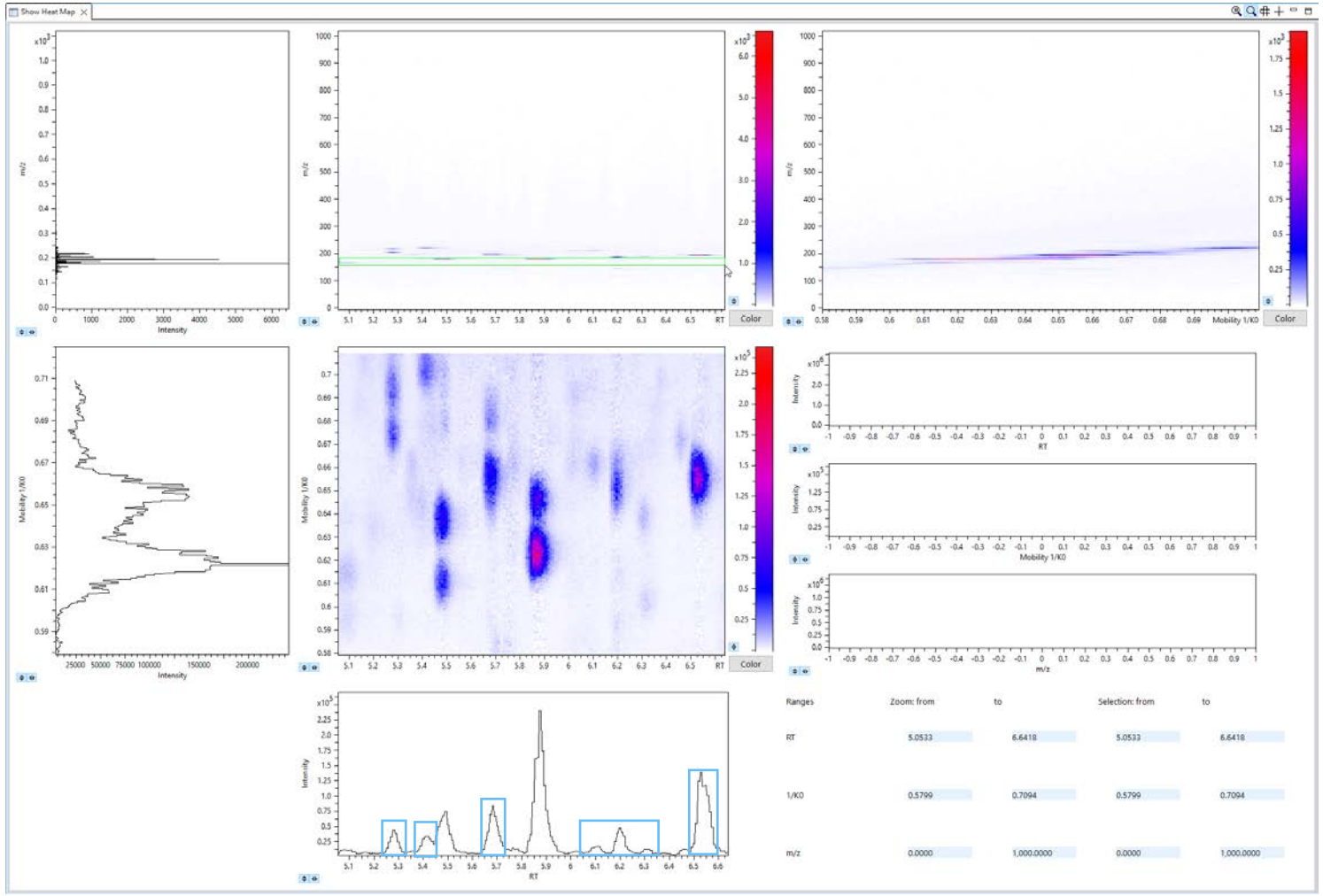
Show Heat Map View - Example



Theobromine

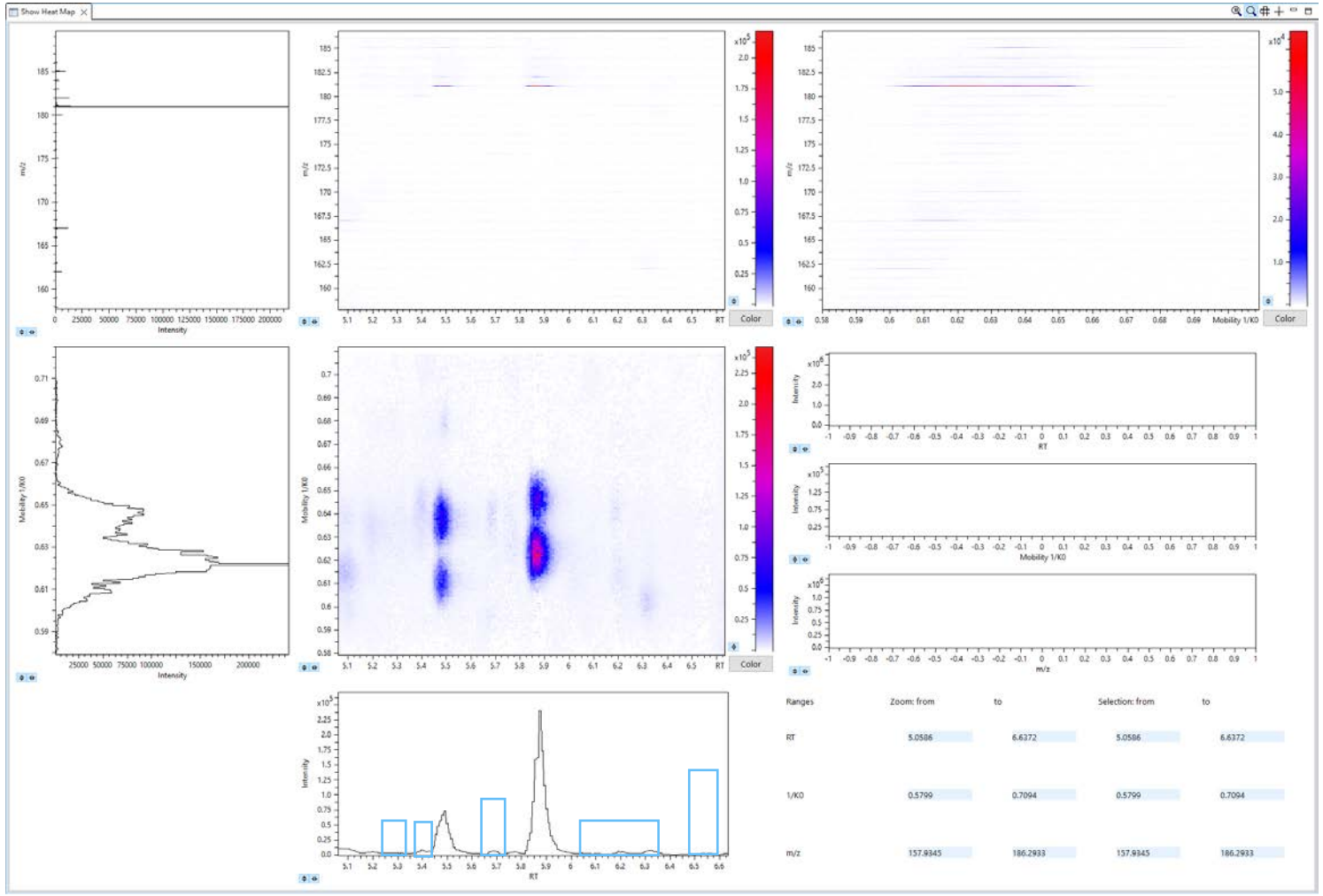


Show Heat Map View – Zooming Data



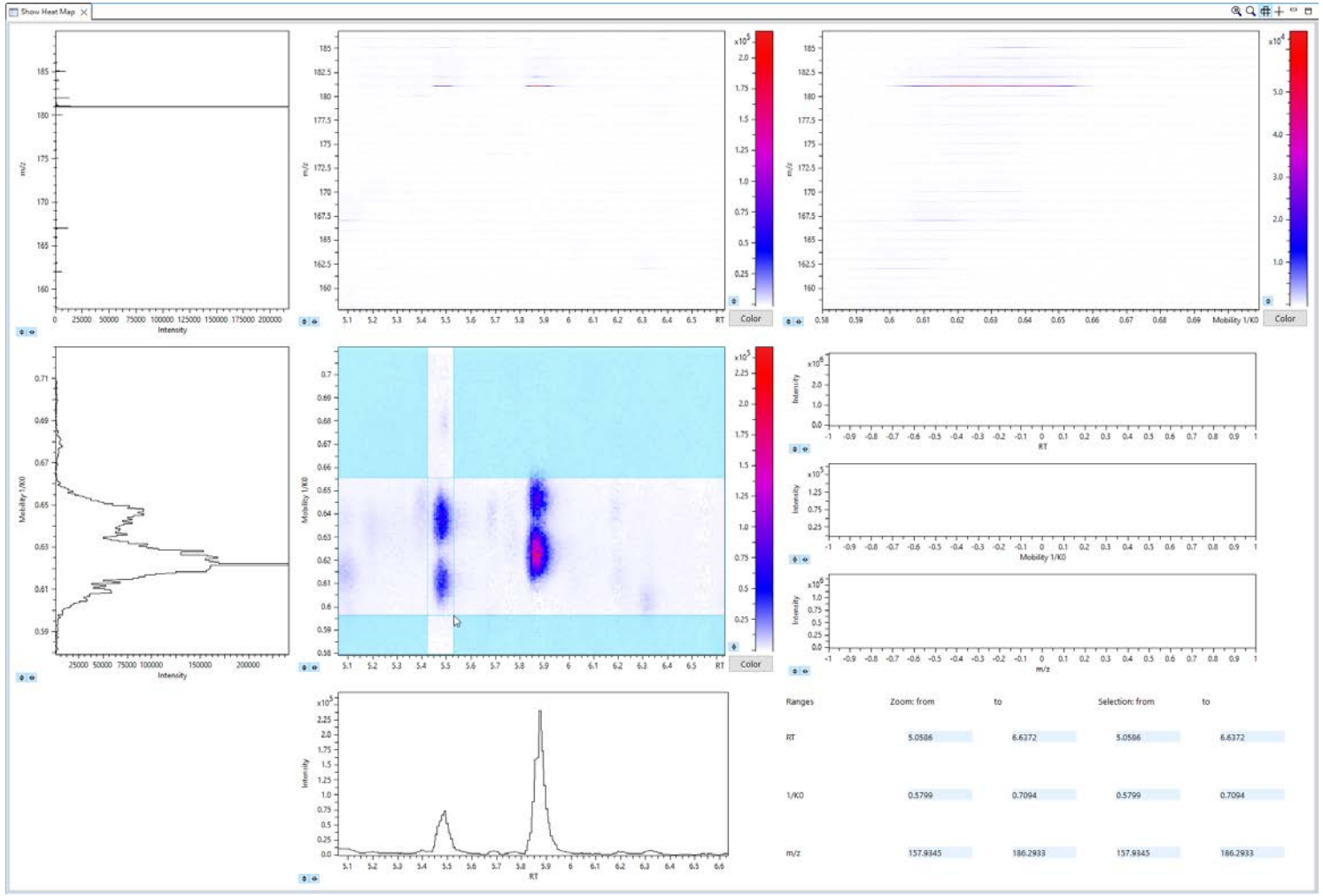
- Zoom into *m/z* range 160 – 190 to get clearer using Zoom mode
- Specify region to zoom by dragging a box with the mouse
- All three projections will be recalculated with the new zoom ranges for *m/z* 160 – 190

Show Heat Map View – Zooming Data Example



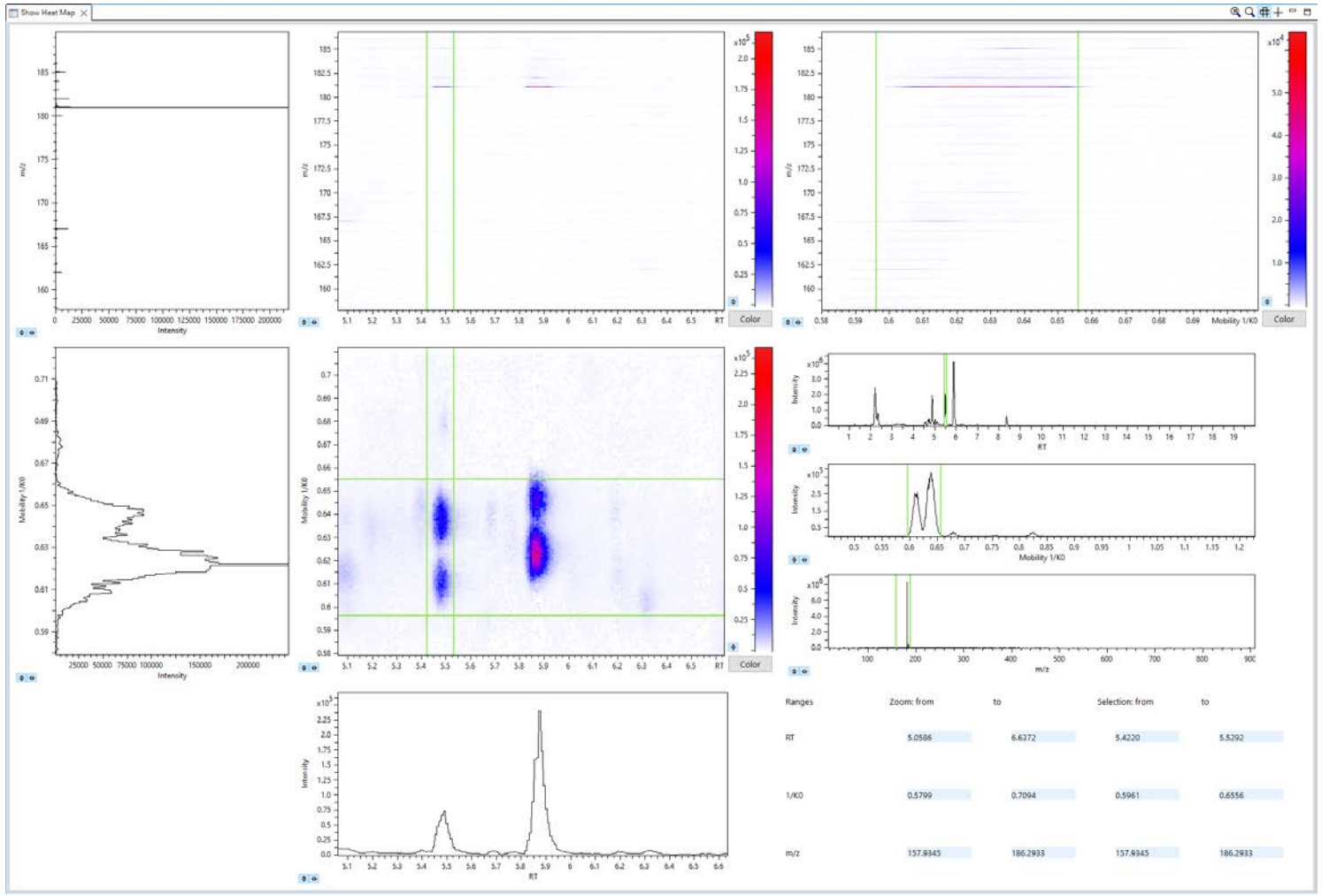
- The projection $1/K_0$ vs RT is now much cleaner containing only data points with *m/z* 160 – 190
- The 1D projection with RT axis shows also less noise compared to the previous slide

Show Heat Map View – Range Selection

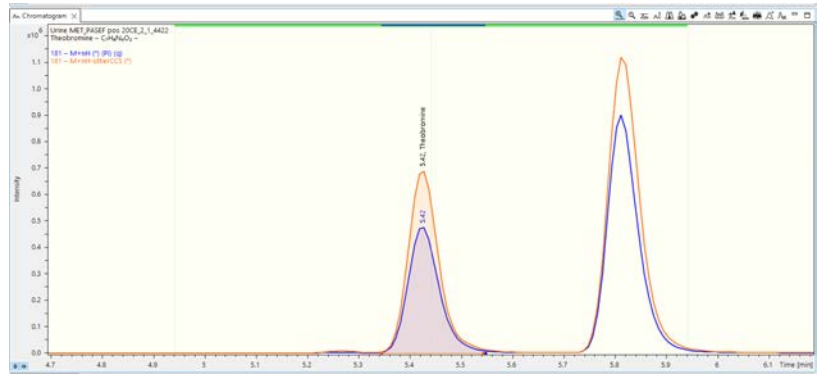


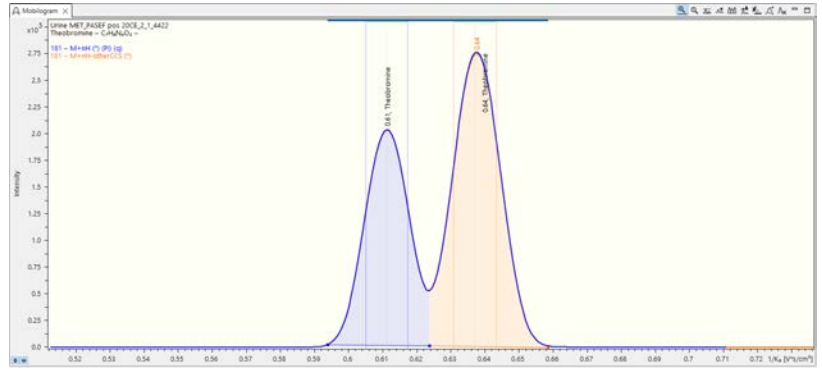
- To get clear EIC, EIM, and average MS spectra for the two signals in range RT 5.45 – 5.25 min and $1/K_0$ 0.595-0.655 [Vs/cm^2] select box selection mode and drag a box with the mouse in region interest

Show Heat Map View – Range Selection (cont.)



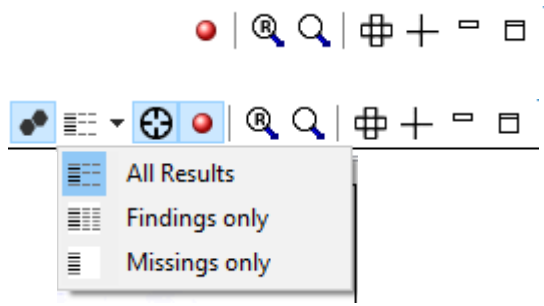
For the selected range EIC, EIM and average MS are calculated which equals to the EIC, EIM of theobromine



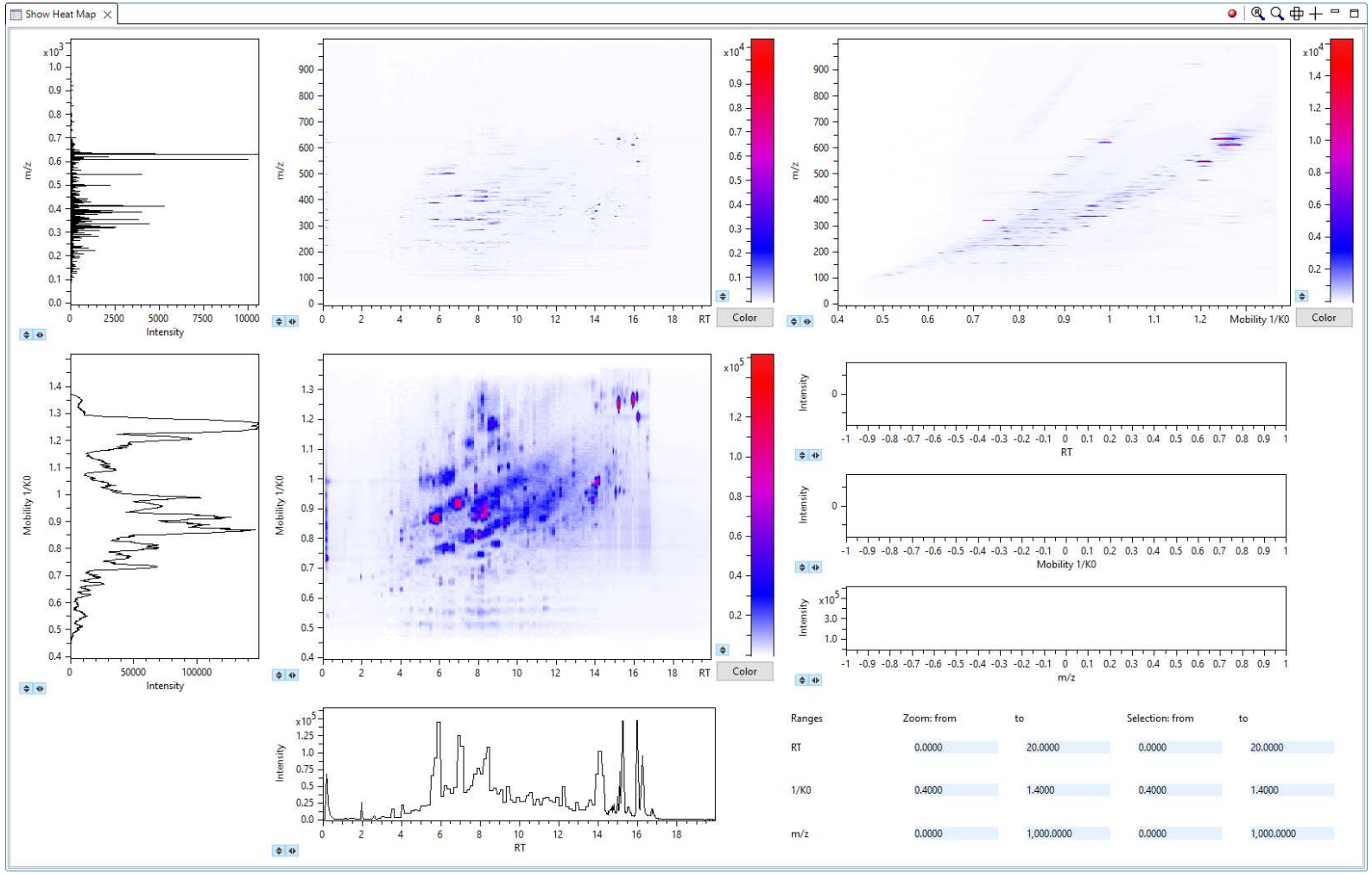


Show Heat Map View – Overlay of Determinations to Projections

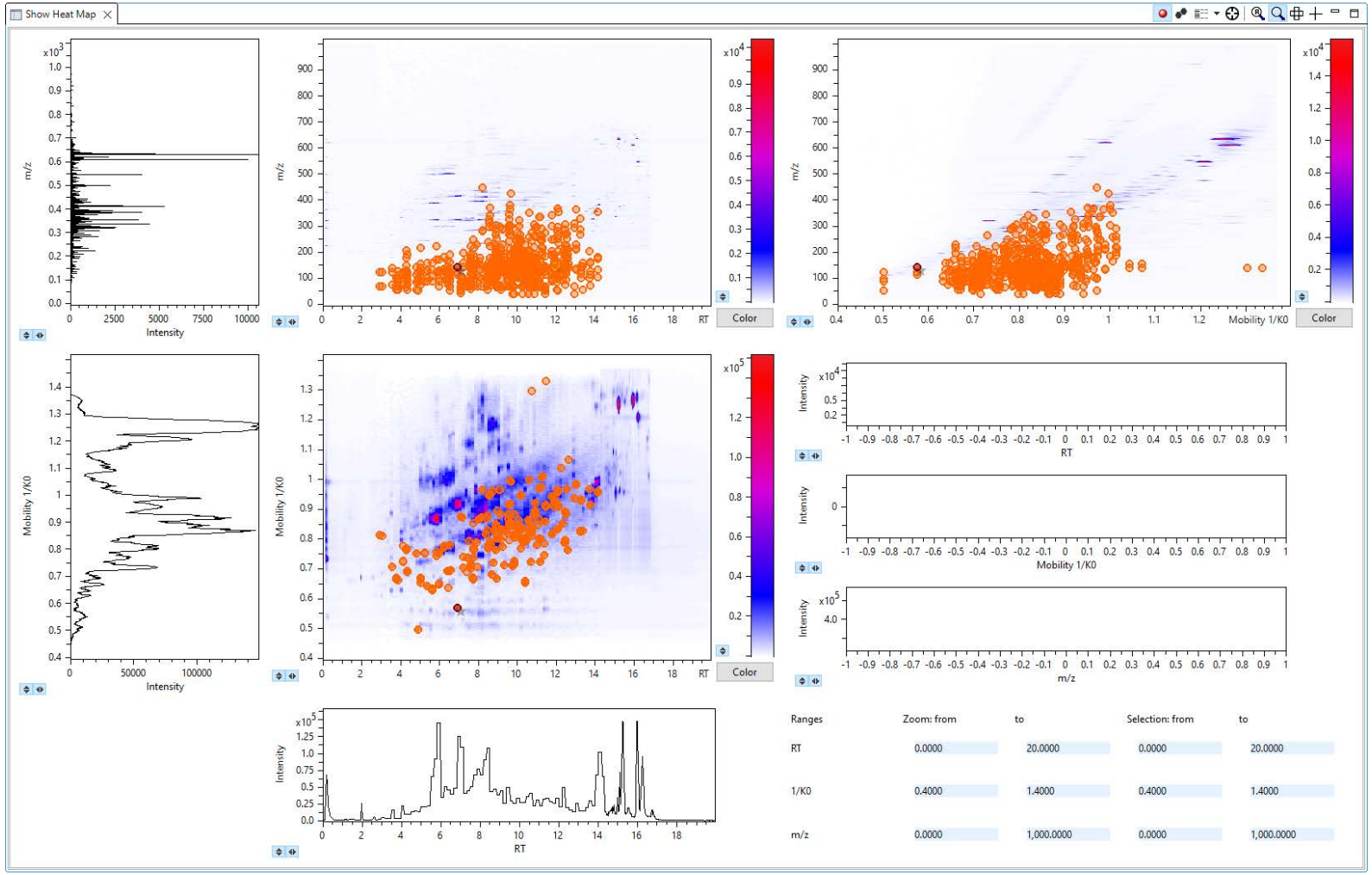
- Add overlay for determinations
- Show principal ion only or marker for each analyte in method
- Show all determinations
- Show only found determinations
- Show only missing determinations
- Select determination



Show Heat Map View – Do Not Overlay Determinations

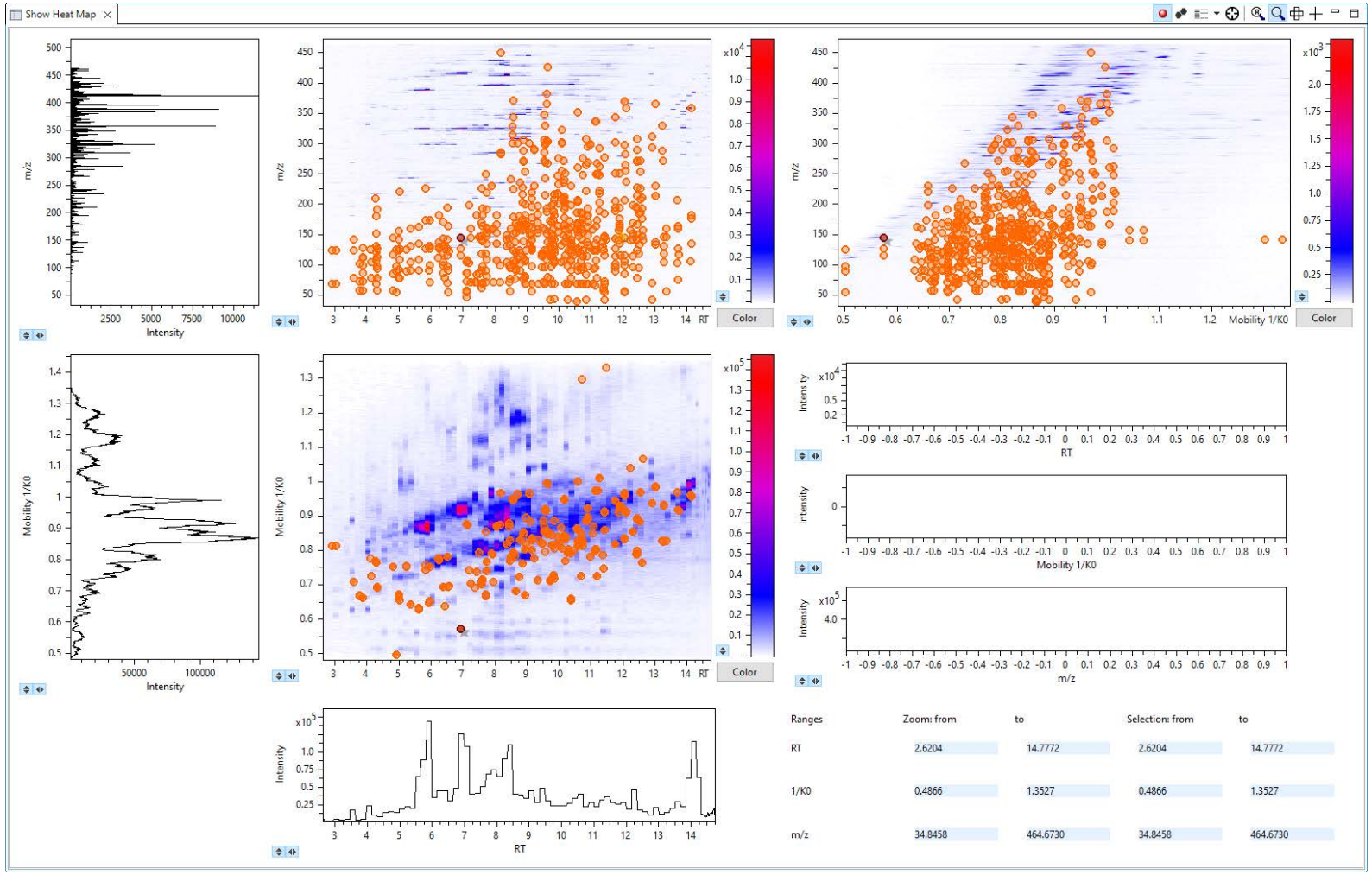


Show Heat Map View – Overlay Determinations

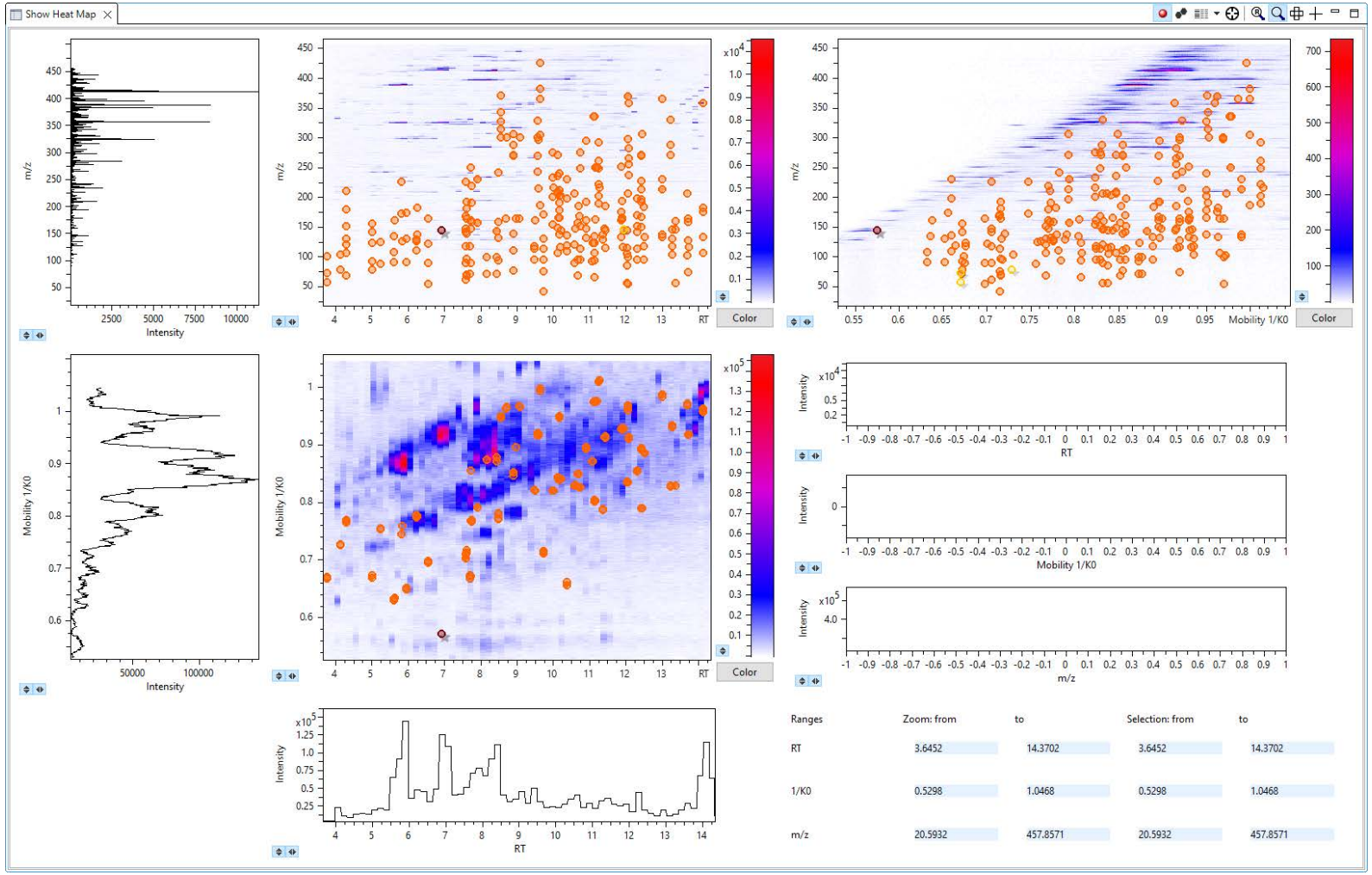


- Show all determinations including missings
- Show all ions

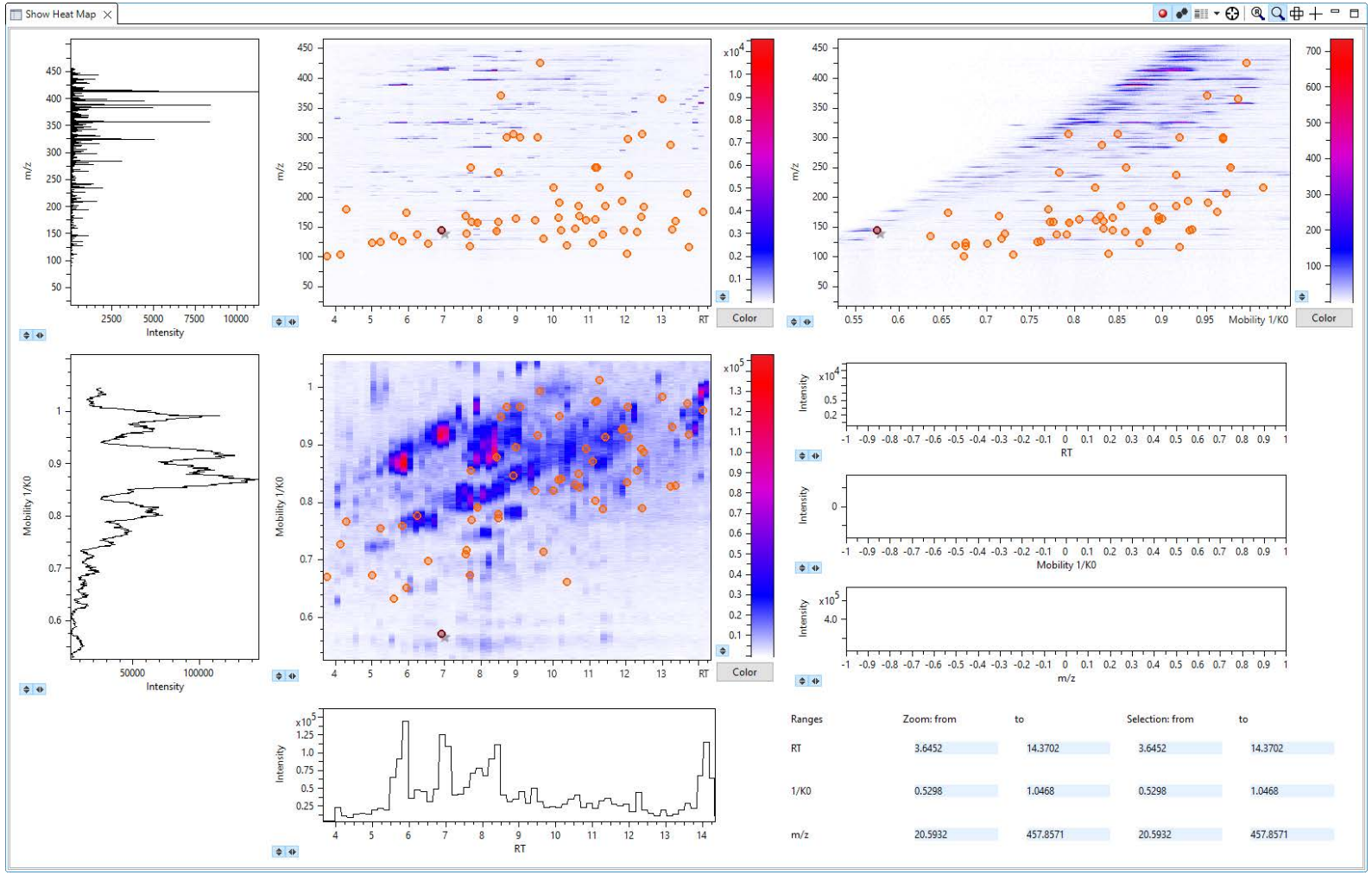
Show Heat Map View – Zoom to Range Where Analytes are Expected



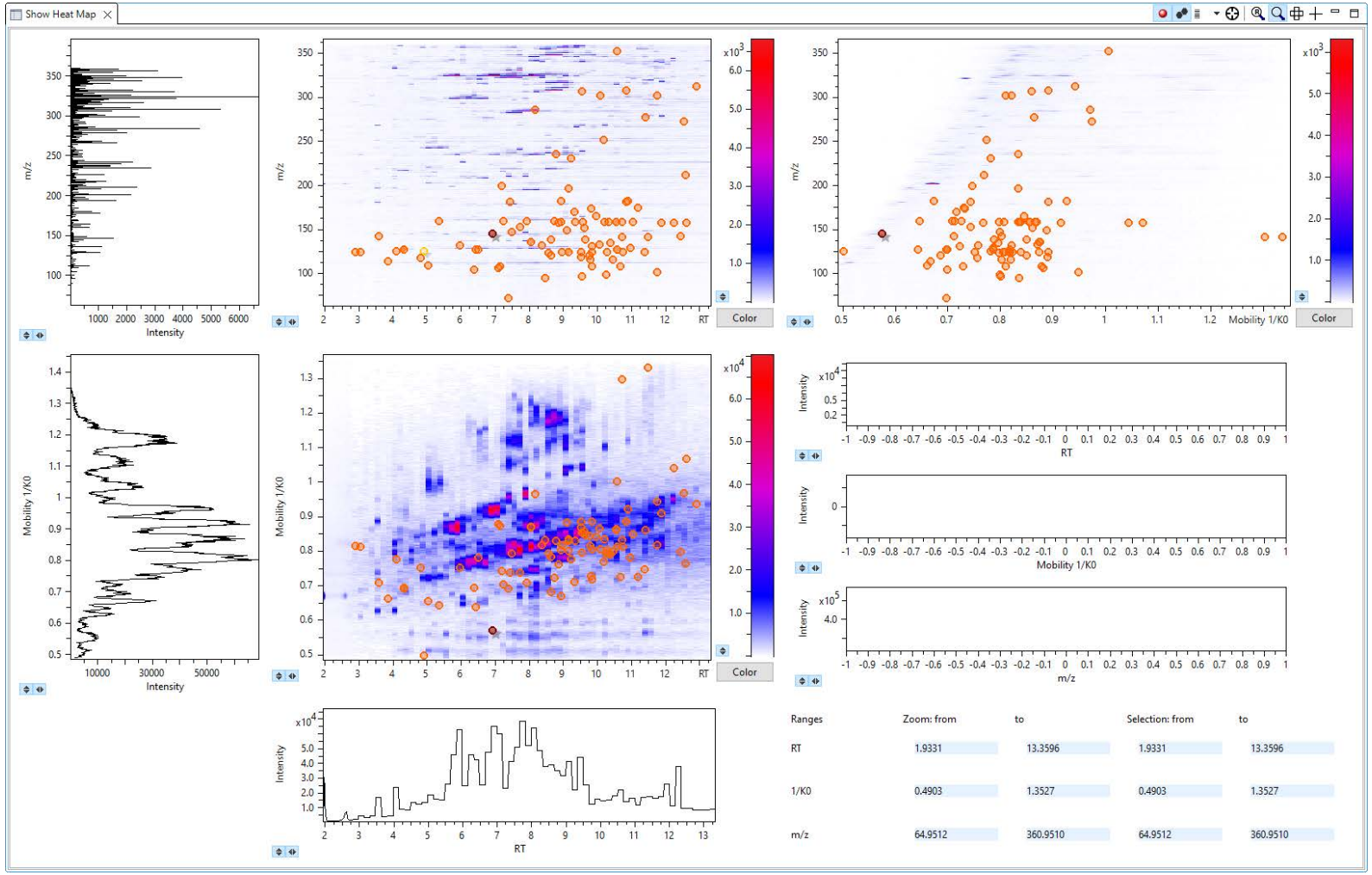
Show Heat Map View – Show Found Determinations Only



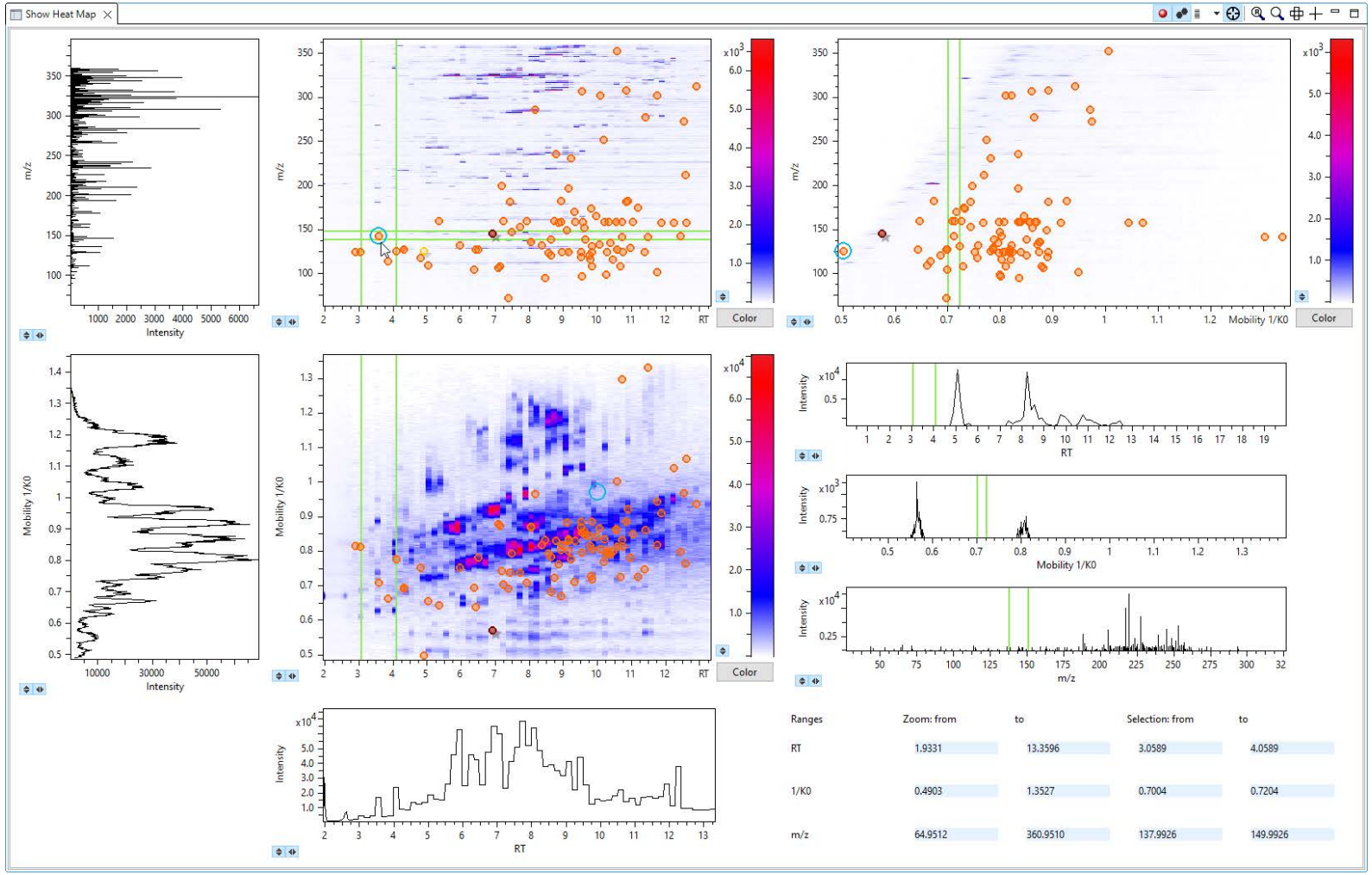
Show Heat Map View – Show Principal Ion Only



Show Heat Map View – Switch to Show Missings

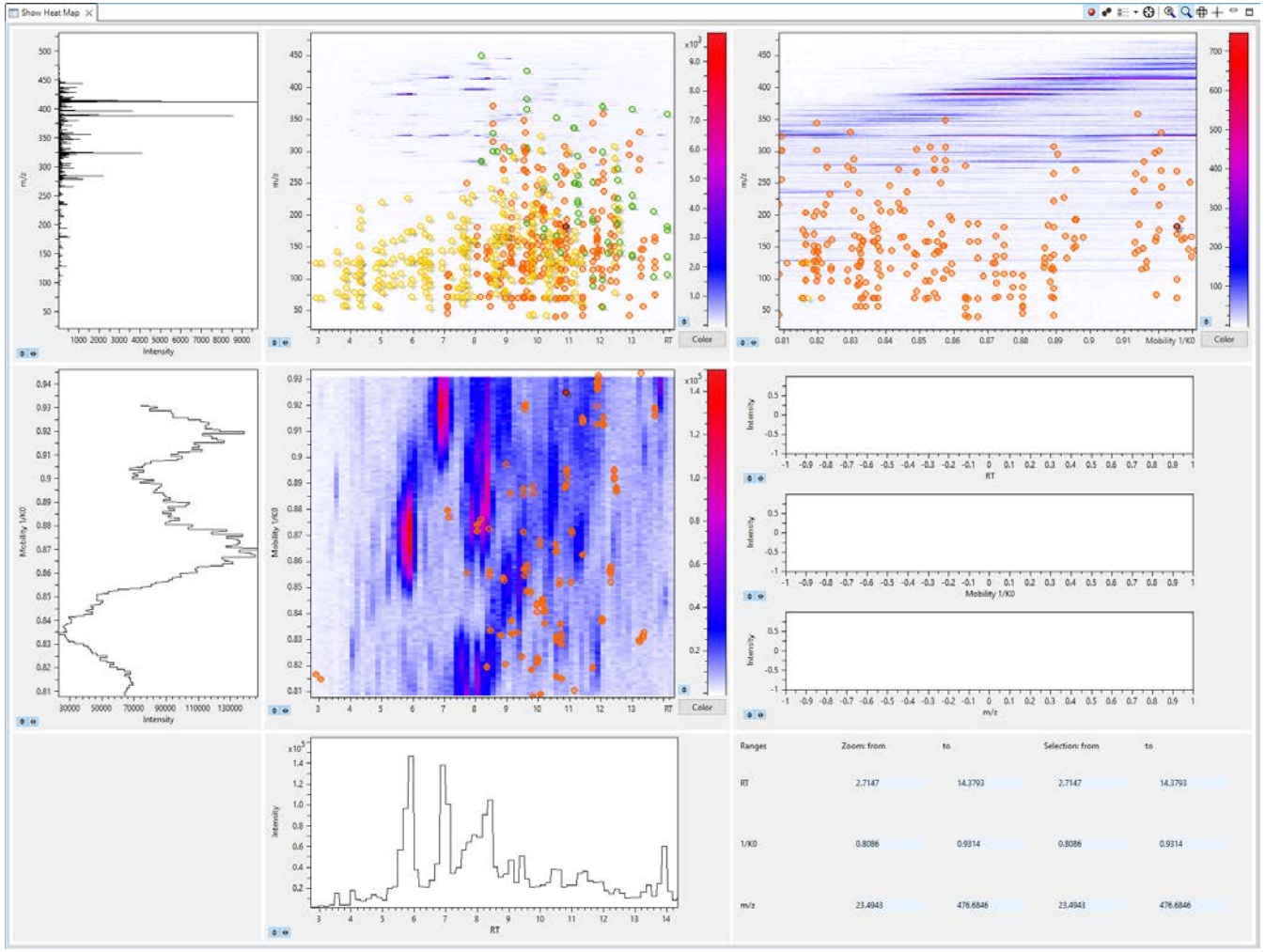


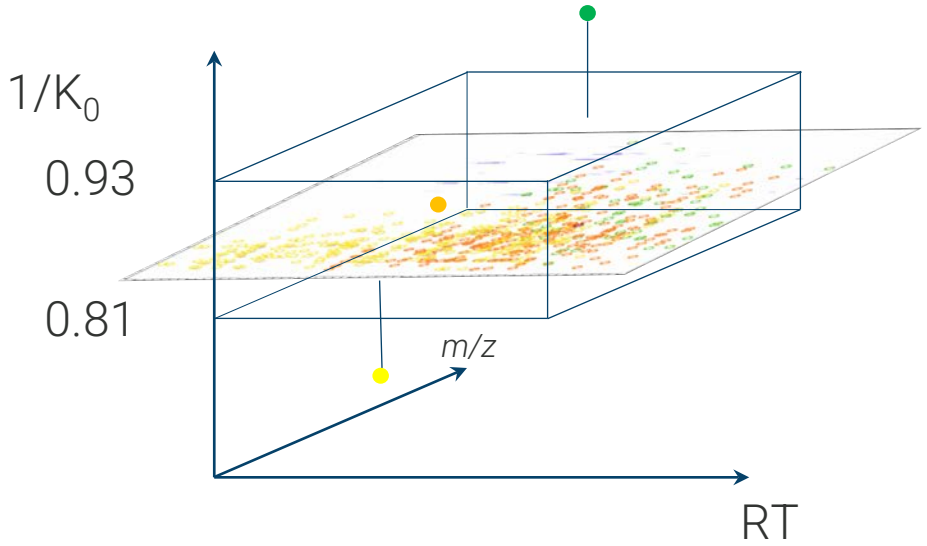
Show Heat Map View – Select a Missing Determination



- Switch on Determination Selection Mode 
- Point with mouse on determination of interest
- Click to select the determination below the mouse
- EIC, EIM and average MS spectrum are shown in the show view pane

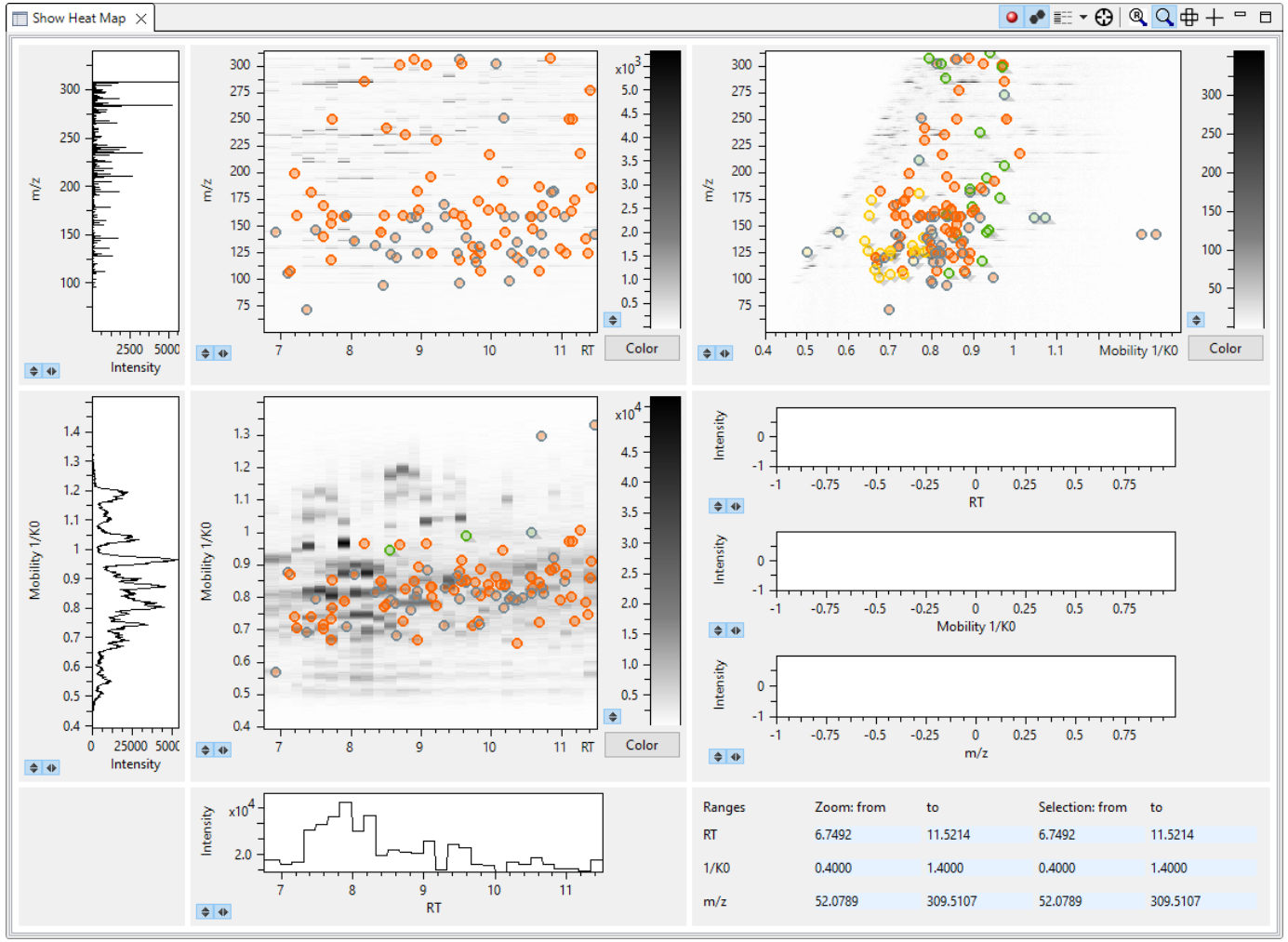
Show Heat Map View - Coding of Determinations above, below or in the pane

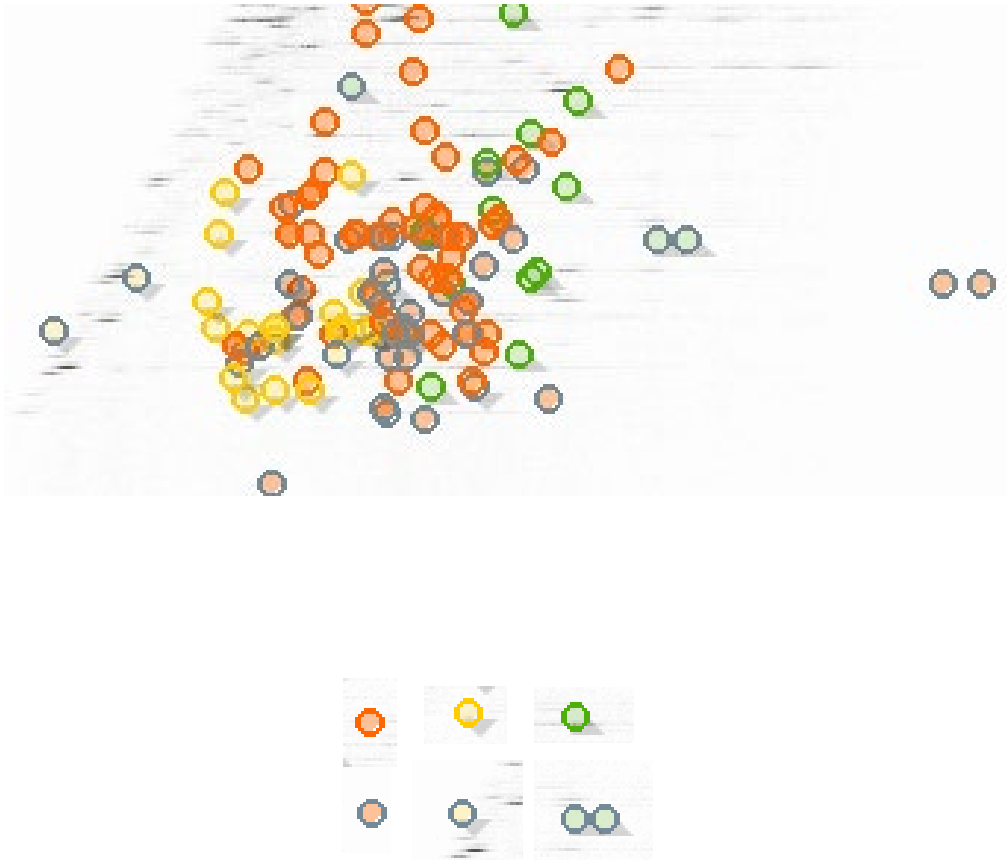




In Determination selection mode press [SHIFT] key and click on determination above or below the pane to shift the vertical zoom range to contain the selected determinations z coordinate and recalculate all projections

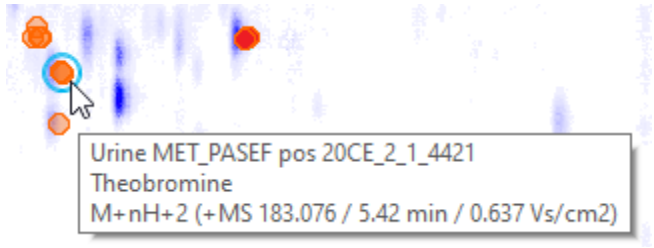
Show Heat Map View – Coding of Missings and Found Determinations





Show Heat Map View – Selecting Determinations – Tooltips

- Additional information for the determination / ion below the mouse is given in a tooltip
  - Name of currently selected data set
  - Name of analyte related to the shown data point
  - Information of ion related to the shown data point
    - Spectrum type (MS, prm-PASEF MS2, bbCID, dia-PASEF)
    - Retention time
    - $1/K_0$

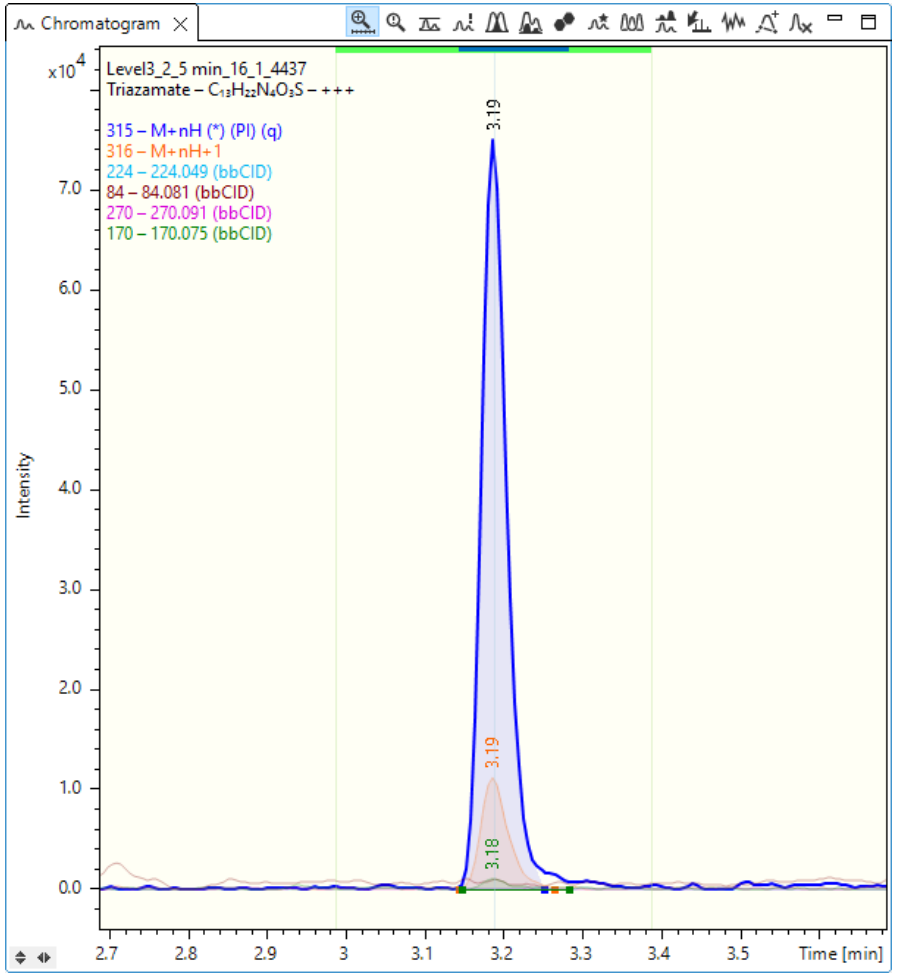


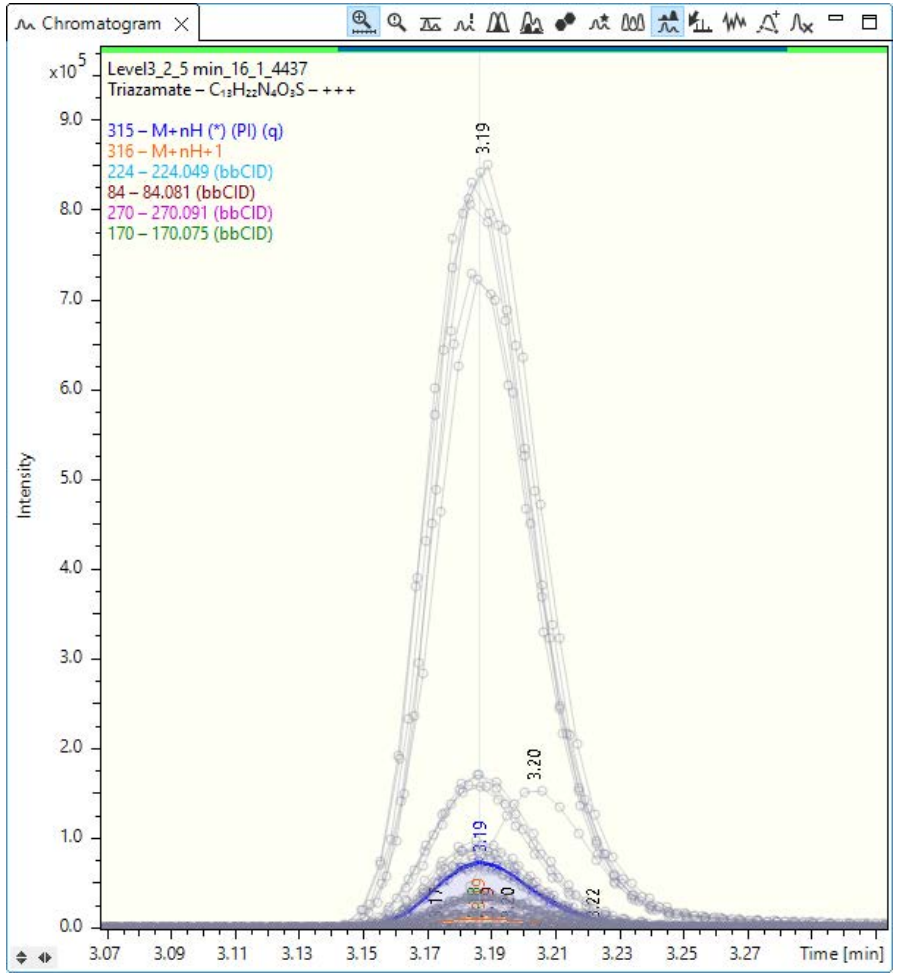
Fit exponentially modified peaks into detected chromatographic / mobilogram peaks

- TASQ offers to fit an exponentially modified peak into a detected chromatographic peak or mobilogram peak
- Select as peak detection mode "Peak Fit"
- In each detected peak an EMG peak will be fitted
- For the resulting EMG peak the derived properties: area, height, peak start and end will be transferred to the results
- There is an option to train an EMG model and store the peak model in the TASQ method
- Typically, the training will be performed with standards of a dilution series
- Subsequently the trained model will be used to reduce the number of parameters to be fitted

Fit exponentially modified peaks into detected chromatographic / mobilogram peaks – Peak Fit Training

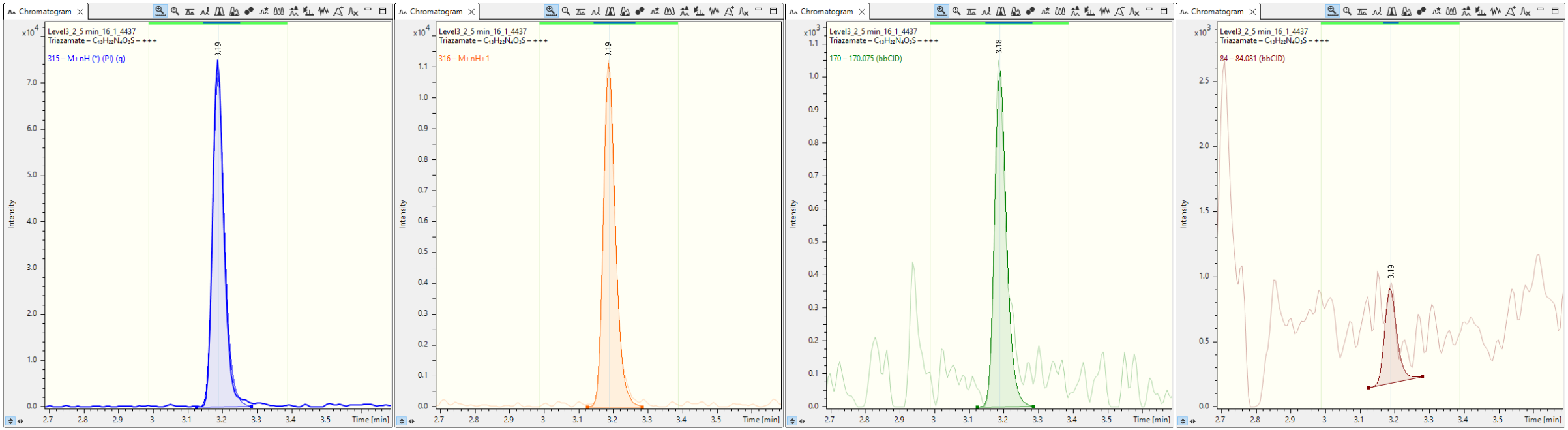
- EMG Peak Fit training is applied to all chromatograms related to an analyte.
- It makes use of all ions.
- And all data sets available in batch.
- By default, calibration samples and quality control samples are used for training.
- An average model is created and stored in TASQ method



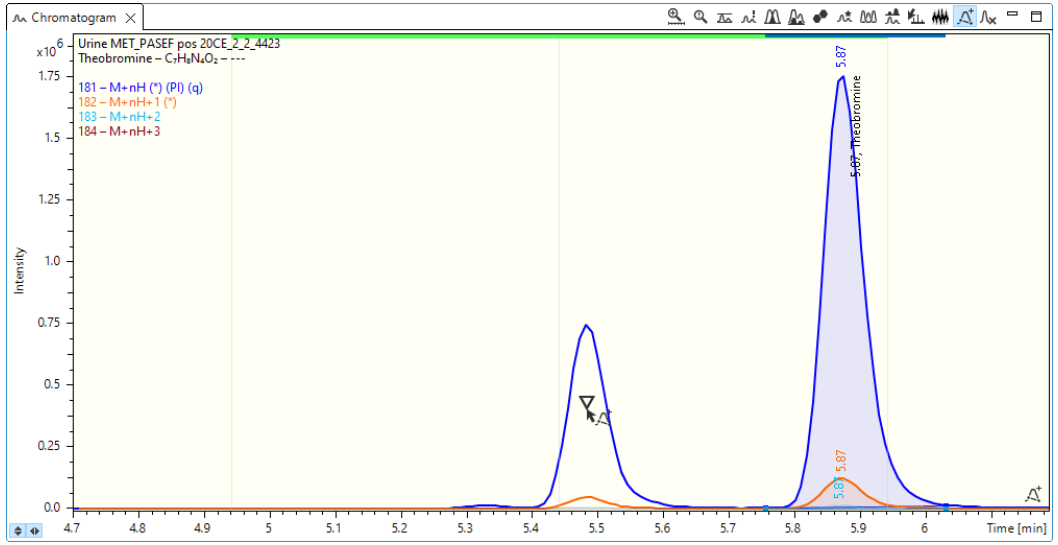


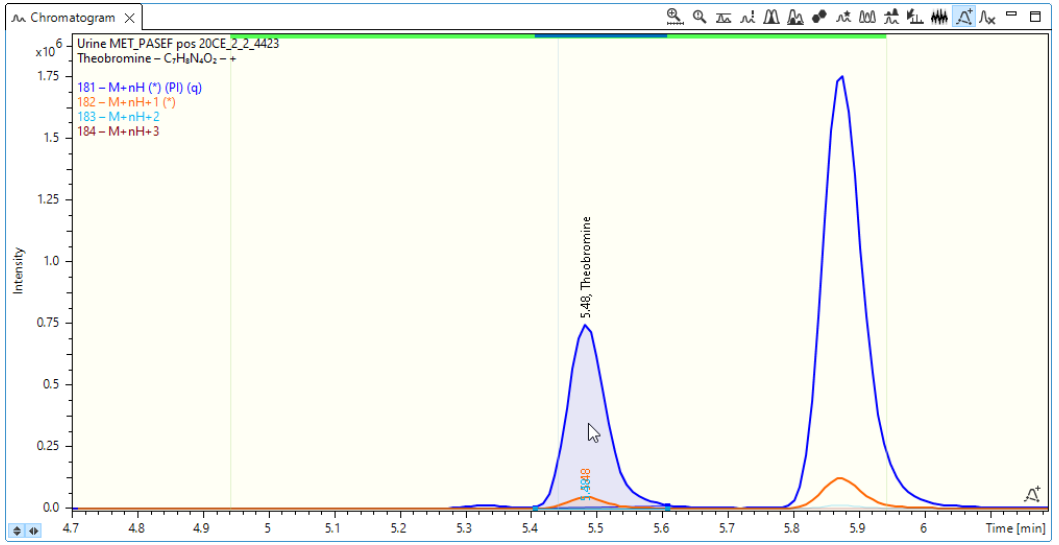
Fit exponentially modified peaks into detected chromatographic / mobilogram peaks

- If an EMG peak model (sigma and tau parameters) is stored in the TASQ method this will be applied for EMG peak fitting.
- The resulting EMG peak fit curve is overlaid in the chromatogram or mobilogram view.
- The derived area, height, peak start and peak end values are transferred to the ion compound results and replaces the values of the classical peak detection algorithm.



New Mode for Manual Integration – PeakPicker





Select manual integration mode
Hover above peak and press [SHIFT] – LMB
Peak will be detected using peak detection algorithm

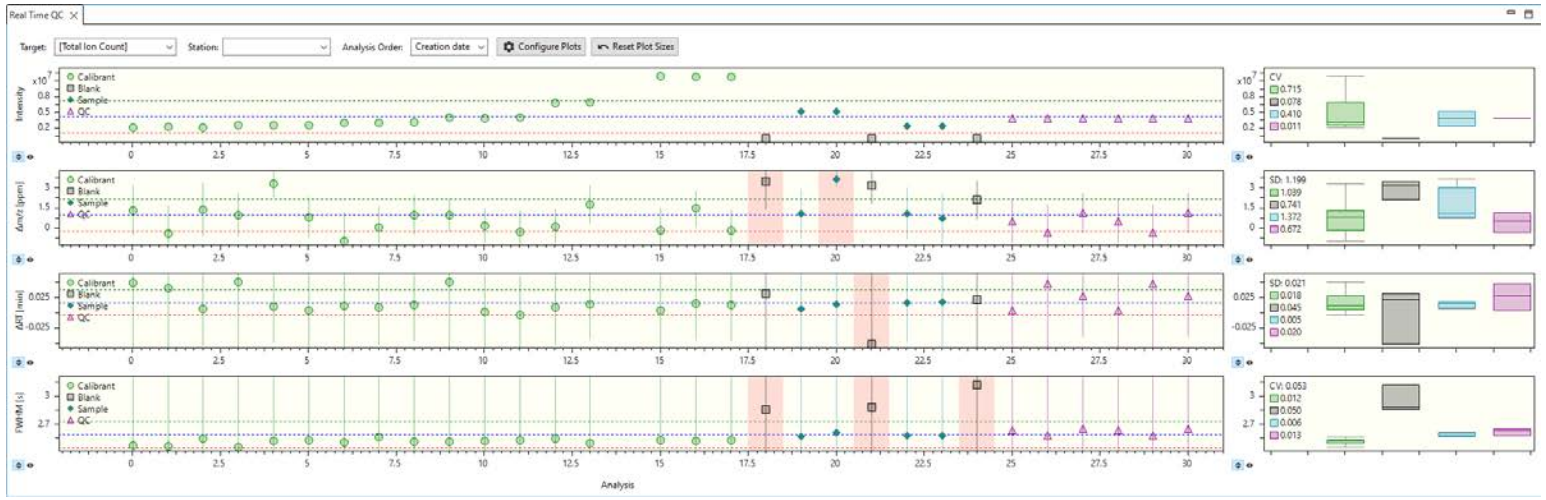
TASQ RealTime QC Monitor

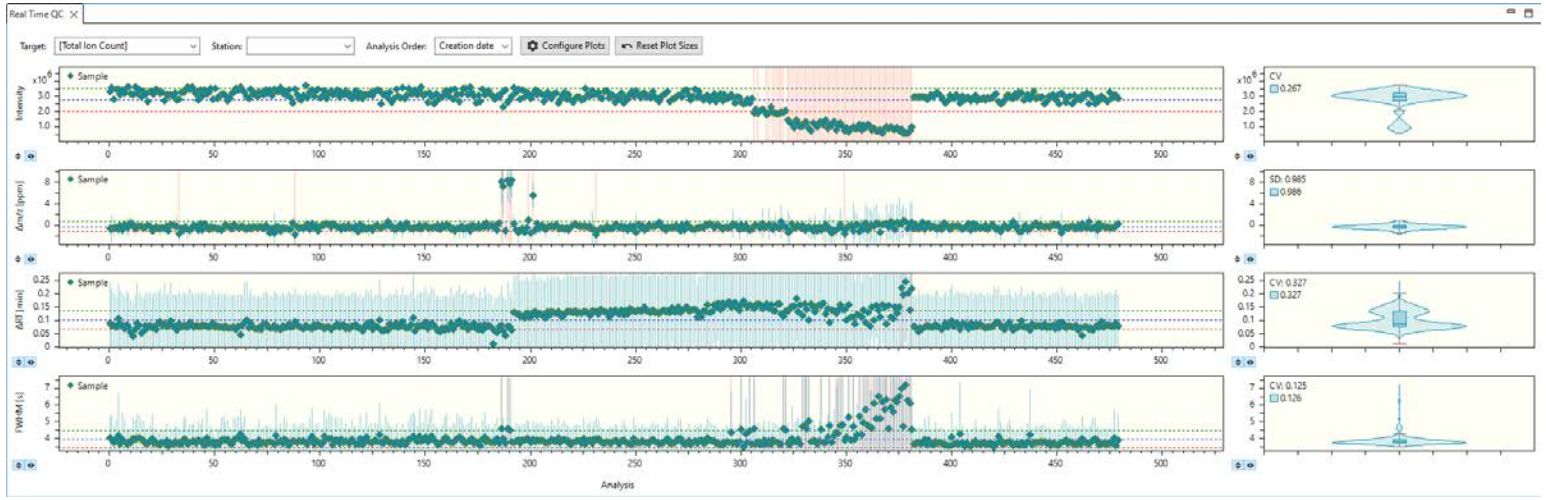
- TASQ RealTime QC Monitor is a tool to overview a currently acquired batch which was setup using the TASQ Batch Setup wizard.
- The Monitor can run on any remote computer connected to the same network containing the compass server and acquisition computers and show the data for a running batch of a selected acquisition computer.
- The presented data will be updated as soon a data set is completely acquired and subsequently processed.
- It will show selected properties for all analytes present in the TASQ method or for a selected analyte.
- The graphical representation of the data will give a feedback on the quality of the batch acquisition and reveals any trends or outliers at a glance.
- Data sets which lies outside a certain margin will be highlighted.

TASQ RealTime QC Monitor

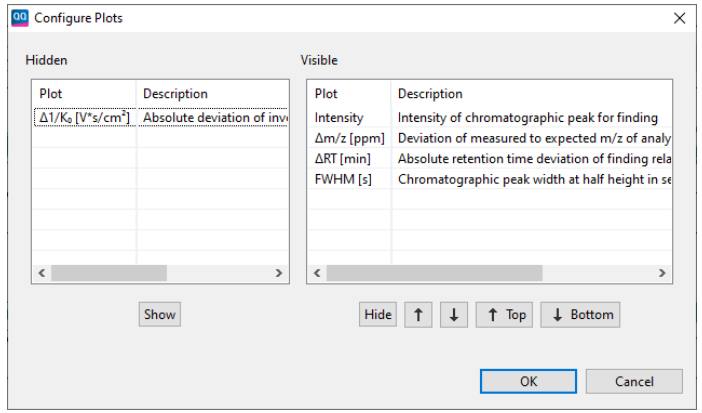
- The set of available properties comprises: Area of detected peaks, retention time accuracy, m/z accuracy, 1/K0 accuracy, and peak width at half height (FWHM).
- For each property, a trend plot and a statistical plot, either as box-whisker or violin plot, are shown.
- Each sample type will be color coded, and the statistical plot will be created for each sample type separately.

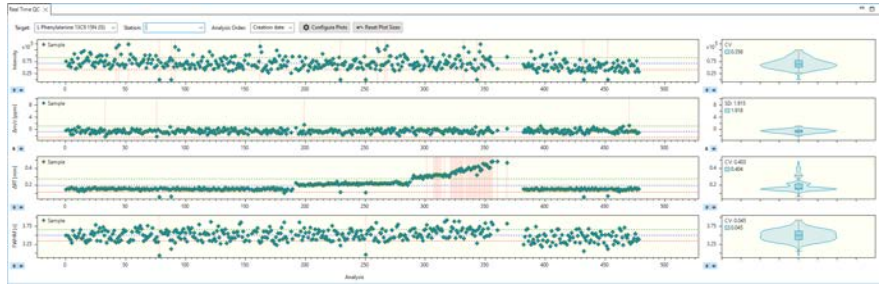
TASQ RealTime QC



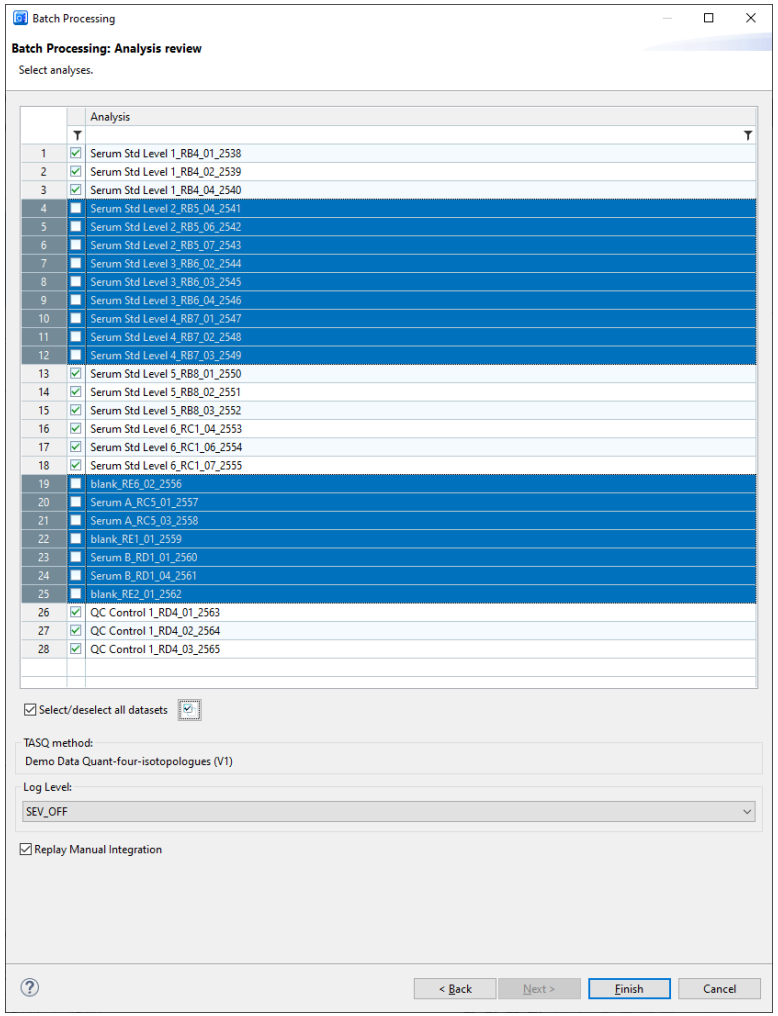


- For each sample type a statistics plot will created. Either as box whiskers plot or violin plot if enough data points are available
- Displayed properties can be selected
- Either show total count (sum of all analytes) or data from a selected analyte



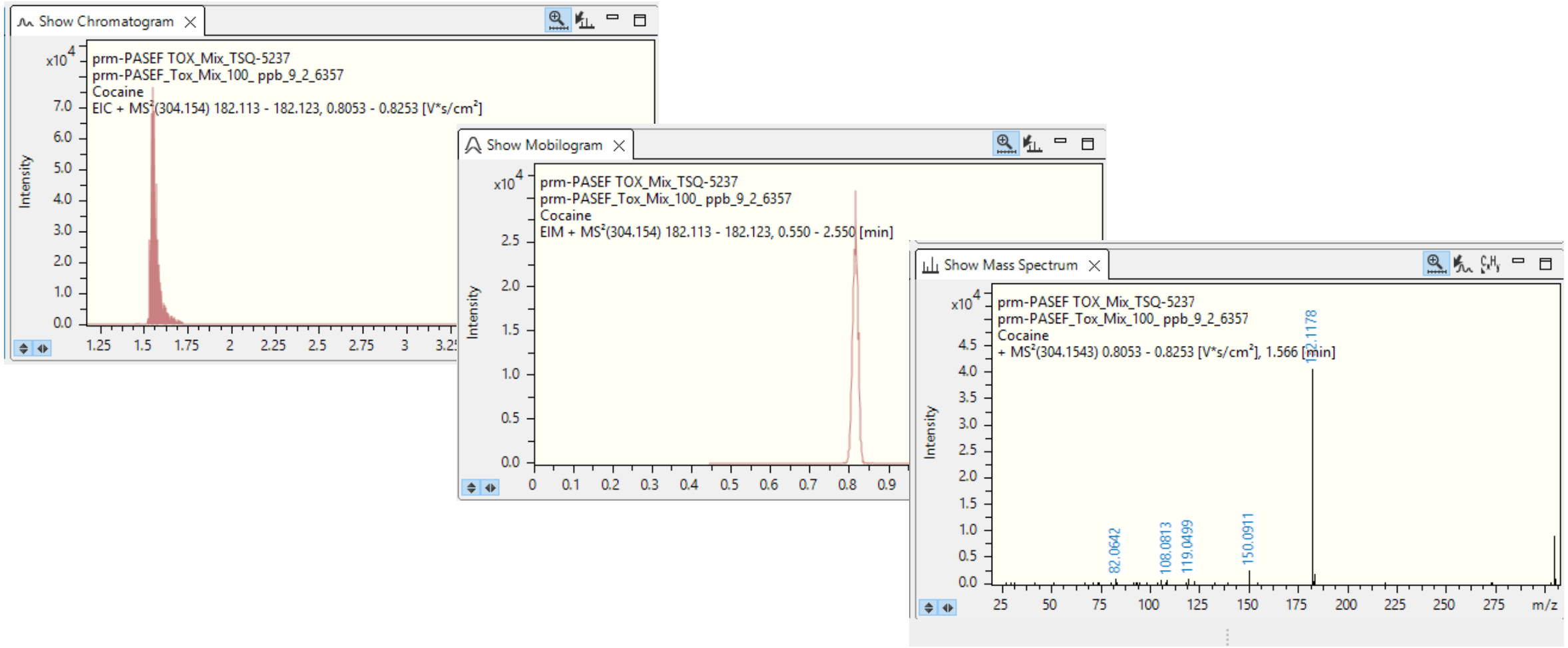


Multi-selection in wizards for selection of enabled for all wizards

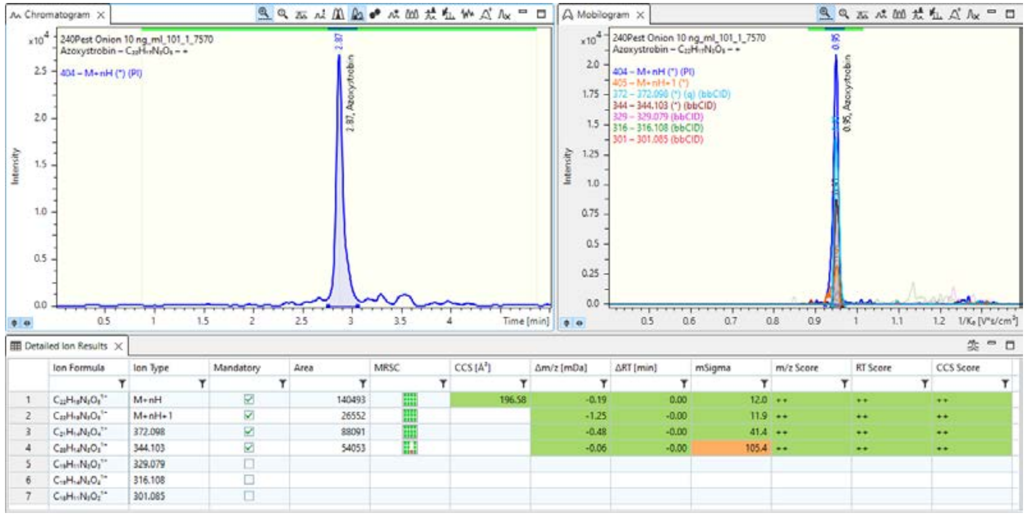


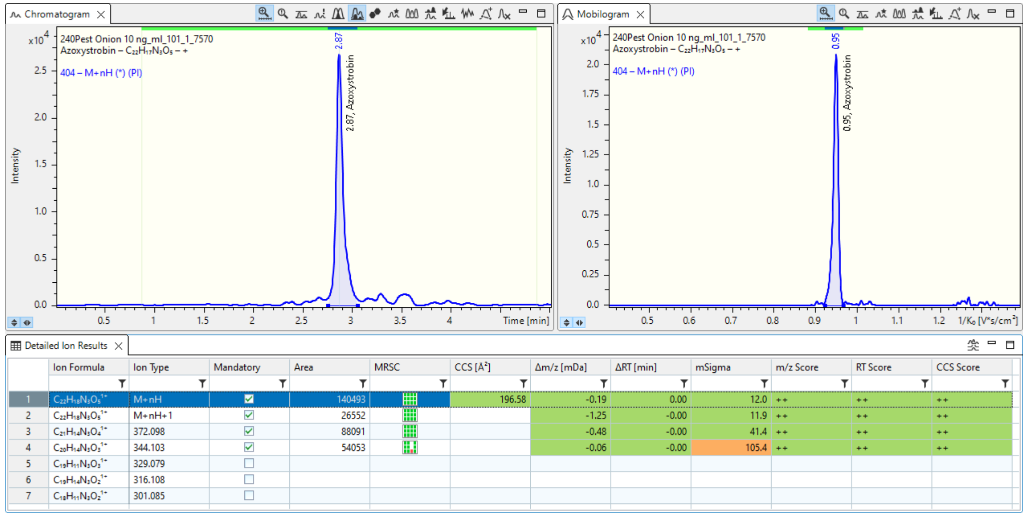
- Select multiple data sets
  - [Shift] LMB
  - [Ctrl] LMB
- Toggle selection state

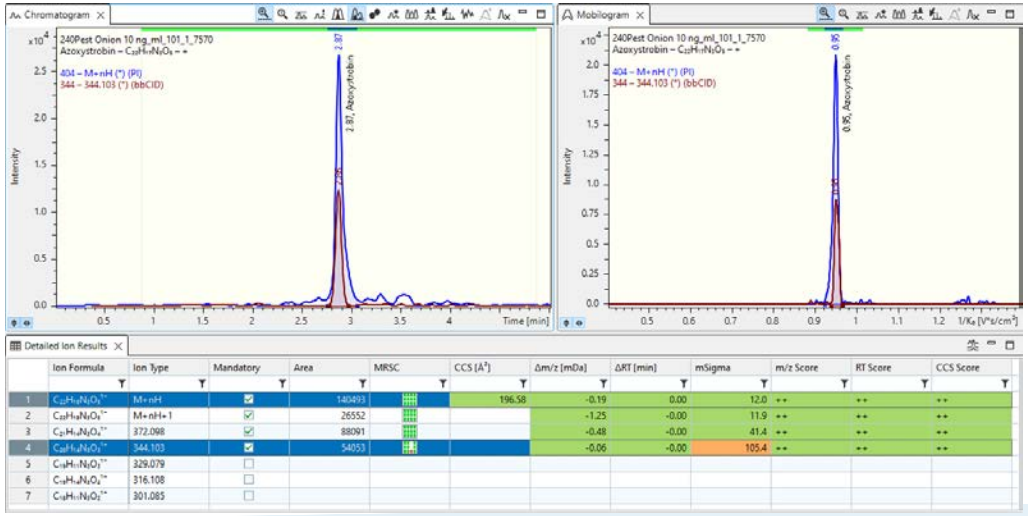
Improved labels in Show … views

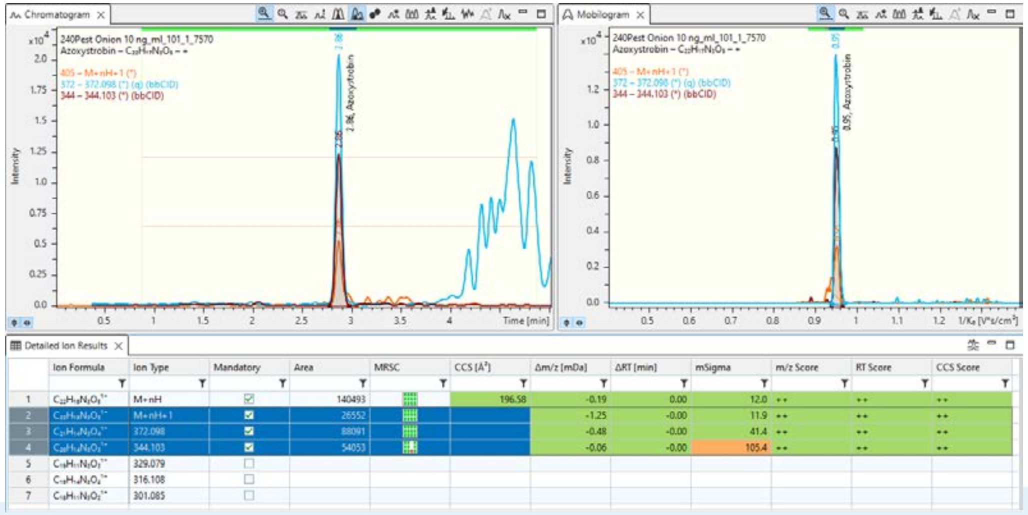


Multi-Selection in Detailed Ion Result view

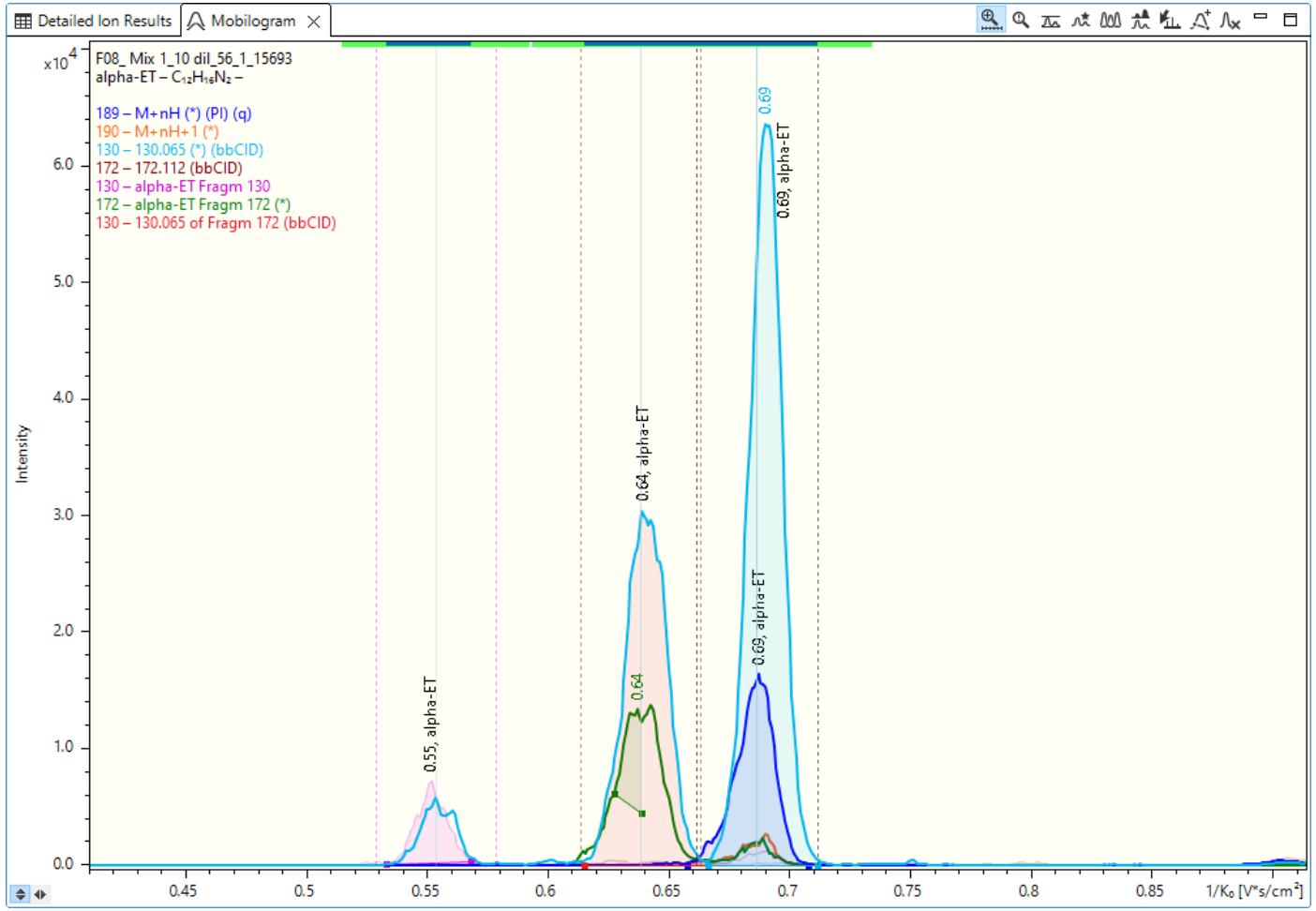




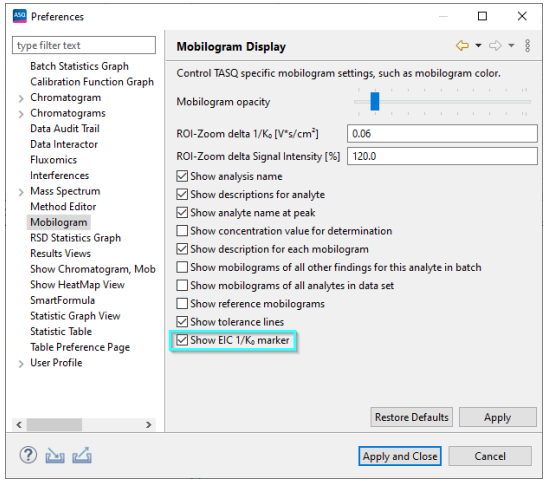




Indicate 1/K_0 Ranges Used for Calculation of EIC

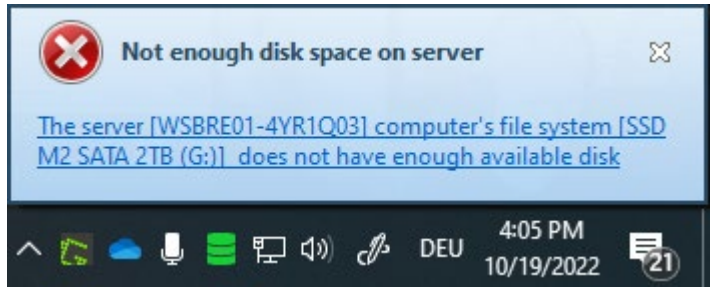


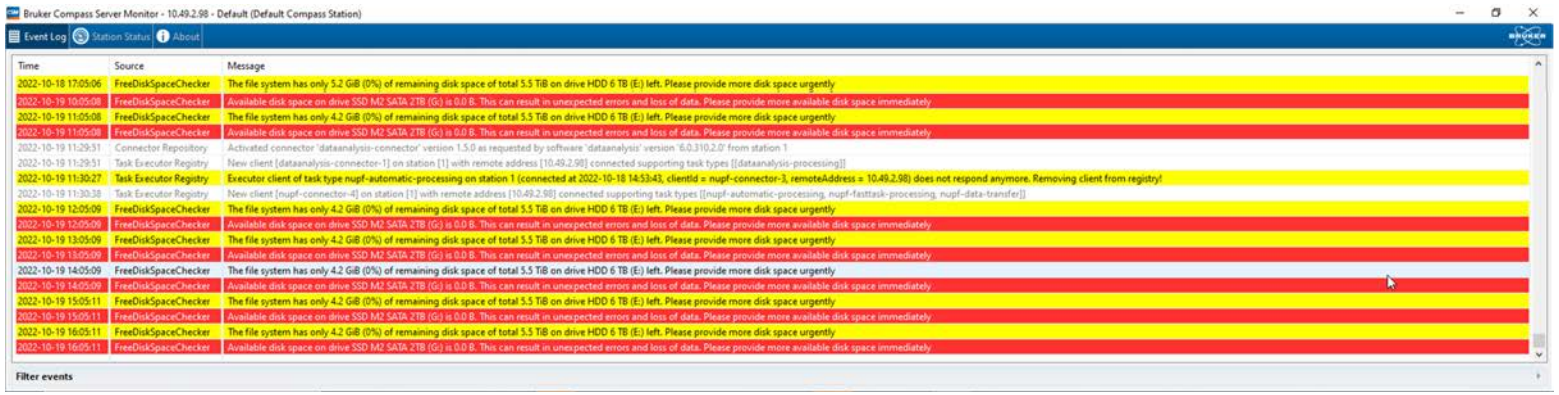
- Dotted vertical lines indicates the 1/K0 ranges which was used for filtering the MS peaks taken into account on building extracte ion chromatograms
- The lines can be overlayed optionally



Warning if Disk is Getting Full

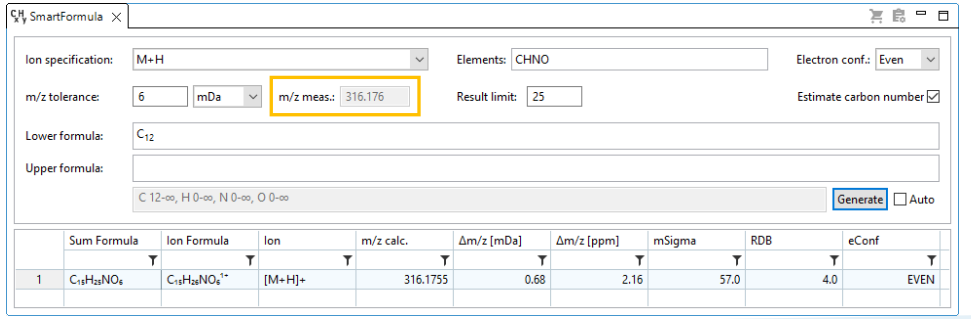
- The compass system checks regulary if the disks where the Compass software and the Compass data base is installed is getting full.
- In case there is no more disk space is available the compass software stops working properly.
- TASQ client will show notifications if Compass platform detects a shortage in disk space and alerts the user that an action has to be taken.
- Additionally corresponding infomation is listed in the log displayed in Compass Monitor client.





Miscellaneous

- Processing of timsTOF data will create BPCs automatically
- BPCs are shown in proper order in chromatogram view.
- In Batch Concentrations view the analyte's tag will be shown additionally. You may sort the table by tag.
- Save method as timsTOF method will suggest a new method name by appending "TIMS" to the current method name.
- An imported batch will be selected in the batch navigator automatically.
- An imported TASQ method will be selected in the method navigator automatically.
- If a user enters audit trail reasons these reasons will be stored and othered the next time again. This is currently only available for manual integration.
- Smart Formula view shows *m/z* value of selected peak more clearly



Miscellaneous

- CCS Score will be calculated also if only $1/K_0$ accuracy is available
- By default, the heap space of TASQ client is increased to 2048 MB.
  - This enables to export large result tables to Excel
- The performance of result tables is improved, and large results can be reviewed properly.
- Guess concentrations in Batch Concentrations view supports different magnitudes of concentration values properly. You may specify concentrations using ppt, ppm, and ppb in the same batch.
- Display of results for analytes with Peak Groups is fixed.

Discontinued Features/Options

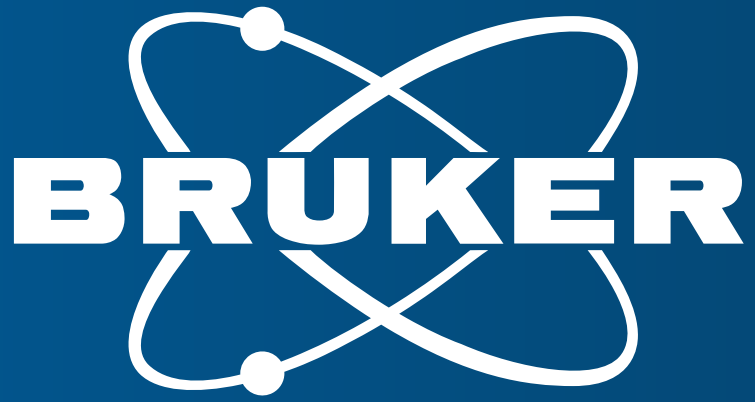
- TASQ does not support creation of prmSettings.sqlite anymore, as timsControl does not support these files. Use export of analyte information as text file instead and import that text file in timsControl to create a prm-PASEF acquisition method.
- There is no option to denoise timsTOF data in TASQ method anymore. Using an older TASQ method, with activated denoising, will ignore that option and processing will be performed without denoising.

Obstacles

- Storage of missed findings was restructured.
  - If you upgrade from a previous TASQ version the results stored in the data base have to be updated to the new scheme.
  - This update of data base may take a long time up to some hours.
  - This depends on the number of data sets stored in the data base.
- Exporting large result tables to Excel may take a long time (few minutes) without any visible reaction of GUI.

Maintenance if Disk is Getting Full

- In case that there is no space left on the disk there the Compass data base is stored these steps can be performed:
  - Install a larger disk and restore the data base on the new disk.
    - Create a backup of the data base.
    - Restore the backup on the new disk.
  - Delete old data sets and results within TASQ client.
    - This may take time and can be done only one data set by another.



Innovation with Integrity