

# What's new in TASQ 2024

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TASQ 2024

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- Method Profile Manager to manage default parameter sets
- Simplified create method, add analyte, add ion wizards making use of method profiles
- Add multiple ions to an analyte in TASQ method
- Overlay of pressure traces in chromatogram(s) view
- Manual integration available in chromatograms view
- Undo all manual integrations at once and get back to the result state after processing
- Batch statistic graph can switch between all determinations of selected analyte, selected data set, or selected batch
- New report layout with graphics for batch statistics
- Cleaner toolbar for chromatogram / mobilogram view
- Performance improvement for quantification
- New Compass 8.0 offers SSL communication

## What's new TASQ 2024

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- Fix for selection of batches for legacy calibration: reduce batches to a time range to reduce the number of possible batches
- Improvements to batch setup wizard
  - Remember positions for calibration, QC, and blank samples in template
- Show missings in batch reports sorted by analytes
- Fill down of peak ranges in method editor fixed
  
- Changes to TASQ RealTimeQC are listed in **What's new TASQ RealTimeQC 2024**

# Method Profile Manager

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For generation of methods from csv file or adding analytes and ions to a method the default parameters are stored in the method profiles.

The Method Profile Manager enables to create, modify, and delete method profile for the various instruments or applications.

The create method wizard, add analyte wizard, and add ion wizard makes use of the method profiles.

In former TASQ versions the mentioned wizards contained many pages for specifying the parameters. These were removed.

Similar to the method editor the same pages for the different categories of parameters are available in the Method Profile Manager



# Method Profile Manager

Method Profile Manager
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	Profile Name	Owner	Instrument Type
1	[compact_microtof]-testwizard	demo	TOF
2	[timstof series negative]	system	timsTOF
3	[timstof series positive]	system	timsTOF
4	[tof series negative]	system	TOF
5	[tof series positive]	system	TOF
6	[triple_quad] (MRM data)	system	TQ
7	[triple_quad] (Fullscan data)	system	TQ
8	Defaultparameter for instrume...	system	TQ
9	Defaultparameter for instrume...	system	TQ

General method settings
Calibration settings
Default Screening Parameter
Ion Type Definition
Default Quantitation Parameters
Number formats
Colors Definition

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

Determination filter: Most mandatories and closest to RT

Chromatogram peak finder mode: Classic

Batch concentration levels: [input] ... [X]

Ion Ratio Signal Type: HEIGHT

Perform smoothing

Perform Denoising (not applied for timsON data)

Max/Min A/H upper limit: 8.000

Minimal datapoints over a peak: 5

Only create chromatogram slices of ± 0.75 [min]

Store MS spectra

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

Signal / Noise Parameters

Algorithm: Classic

S/N filter: 3.000

Surrogate noise: 1.000

# Method Profile Manager

General method settings | Calibration settings | **Default Screening Parameter** | Ion Type Definition | Default Quantitation Parameters | Number formats | Colors Definition

Perform mass calibration and replace existing one

Reference Mass List:  ...

Retention time range Start:  min End:  min

Note: If start and end are set to '0.0' the complete retention time range is taken for creating the spectrum used for calibration.

Intensity threshold:  m/z range ±:  Da

Perform Lock mass calibration

Reference Lock Mass:  ...

Intensity threshold:  m/z range ±:  Da

General method settings | Calibration settings | **Default Screening Parameter** | Ion Type Definition | Default Quantitation Parameters | Number formats | Colors Definition

Screening Parameters

EIC Width ±:  mDa

m/z Scoring Narrow ±:  ppm

m/z Scoring Wide ±:  ppm

mSigma Tolerance:

mSigma Scoring Narrow:

mSigma Scoring Wide:

Retention Time [min]

RT Tolerance ±:

RT Scoring - Narrow ±:

RT Scoring - Wide ±:

Integration Parameters

Area abs threshold:

Height abs threshold:

Min Peak Valley [%]:

Sensitivity [%]:

Smoothing Parameter

Smoothing width [s]:

Smoothing cycles:



# Method Profile Manager

General method settings | Calibration settings | Default Screening Parameter | Ion Type Definition | Default Quantitation Parameters | Number formats | Colors Definition

Adduct: M+nH | Isotopologue: most abundant | most abundant: mandatory | 2nd most abundant: mandatory | 3rd most abundant: opt | 4th most abundant: opt | Add Ion Definition

	Adduct	Isotopologue	monoisotopic	most abundant	2nd most abu...	3rd most abund...	4th most abund...
1	M+nH	monoisotopic					
2		monoisotopic					

Delete Definitions

Regarding isotopes the ratios are calculated and with a tolerance of 30% entered in the method.

General method settings | Calibration settings | Default Screening Parameter | Ion Type Definition | Default Quantitation Parameters | Number formats | Colors Definition

Quantitation Parameters

Origin: ignore | Signal: Area | Weighting: none | Function: linear



# Method Profile Manager

General method settings | Calibration settings | Default Screening Parameter | Ion Type Definition | Default Quantitation Parameters | Number formats | Colors Definition

Mass error (ppm, mDa, ...)	<input type="text" value="2"/>
Mass (m/z measured, m/z expected, ...)	<input type="text" value="4"/>
RT, relative RT	<input type="text" value="2"/>
mSigma	<input type="text" value="1"/>
Intensity	<input type="text" value="0"/>
Area	<input type="text" value="0"/>
Ratios (relative Area and Intensity)	<input type="text" value="3"/>
Quantity / Concentration	<input type="text" value="1"/>
Injection volume	<input type="text" value="0"/>
Recovery / Accuracy	<input type="text" value="2"/>

General method settings | Calibration settings | Default Screening Parameter | Ion Type Definition | Default Quantitation Parameters | Number formats | Colors Definition

Analyte Score

- Background: Invalid
- Background: Tentative Identification
- Background: Medium Identification
- Background: Strong Identification

Analytes

- Found in Analysis
- Missed in Analysis

Ion Colors

- Background: Narrow
- Background: Wide
- Background: Outside
- Foreground: Narrow
- Foreground: Wide
- Foreground: Outside

Other Colors

- Background: Rel. quantity and quantity result by legacy, surrogate or single point calibration



# Add Multiple Ions To An Analyte In TASQ Method At Once

Multiple ions can be added at once to an analyte in a TASQ method.

Copy and paste, e.g., a MS peak list from DataAnalysis into the Add Multiple Ions wizard.

Assign clipboard import to table columns

Assign imported clipboard data to table columns for inserted.  
Assign the columns from the imported clipboard data to the corresponding columns.

Column of m/z: COL\_1  
Column of Intensity: COL\_2  
Default Spectrum Type: FULLSCAN

Column of Ion formula:   
Column of Charge:   
Default Charge when missing: 1

First row in table below is a header row

COL_0	COL_1	COL_2
#	m/z	I
1	42.0342	17405
2	49.4997	5308
3	54.4976	3986
4	56.9649	2534
5	58.5049	6488
6	59.0493	5913
7	59.0603	3726
8	60.0446	1763
9	61.0076	11295
10	62.0242	1922
11	64.0158	8872
12	67.5101	4234
13	68.5004	3442
14	68.9941	12956
15	69.9946	1894
16	70.0128	19304
17	71.0296	2803
18	72.9372	11156
19	73.0649	2298
20	74.0600	1851
21	74.9375	2229
22	75.0107	1661

OK Cancel

Add multiple ions

Add multiple ions from table below to selected analyte Alprazolam (C17H13ClN4)  
Fill the table with ion informations and select a method parameter profile.

	Add	Ion	Ion formula	m/z	Charge	Spectrum type	Precursor m/z	Intensity	Most abundant	2nd r
1	<input checked="" type="checkbox"/>	271.0620		271.0620	1	FullScan		1644107		
2	<input checked="" type="checkbox"/>	273.0594		273.0594	1	FullScan		504300		
3	<input checked="" type="checkbox"/>	272.0655		272.0655	1	FullScan		265438		
4	<input type="checkbox"/>	622.0257		622.0257	1	FullScan		260459		
5	<input checked="" type="checkbox"/>	158.9611		158.9611	1	FullScan		136401		
6	<input checked="" type="checkbox"/>	276.0936		276.0936	1	FullScan		128519		
7	<input checked="" type="checkbox"/>	114.0912		114.0912	1	FullScan		93782		
8	<input checked="" type="checkbox"/>	274.0627		274.0627	1	FullScan		87693		
9	<input type="checkbox"/>	445.2755		445.2755	1	FullScan		63107		
10	<input checked="" type="checkbox"/>	186.9557		186.9557	1	FullScan		56843		
11	<input checked="" type="checkbox"/>	87.0043		87.0043	1	FullScan		52718		
12	<input checked="" type="checkbox"/>	130.0078		130.0078	1	FullScan		51734		

Select/deselect all rows

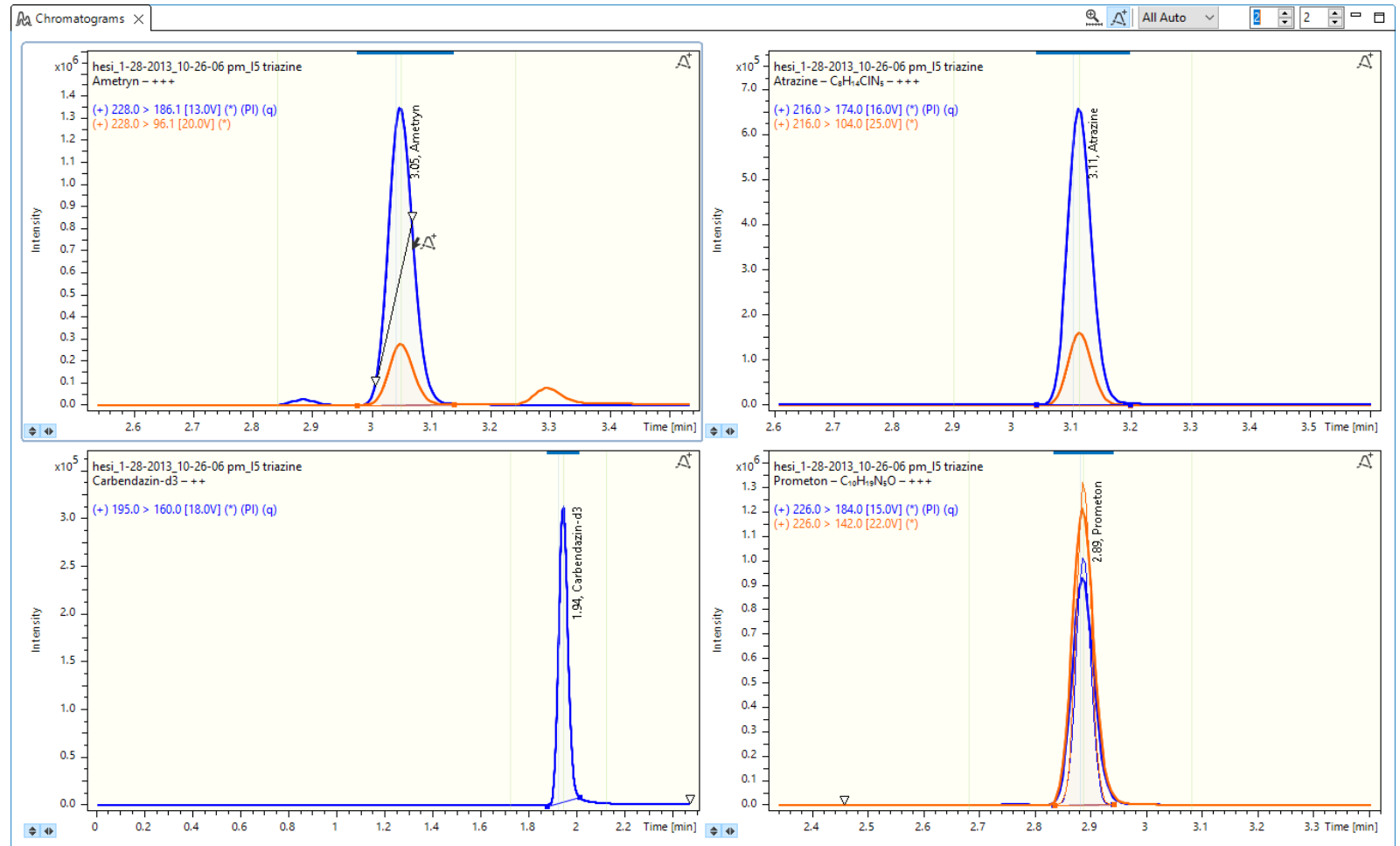
Method Parameter Profiles

[compact\_microtof]-testwizard  
[tof series negative]  
[tof series positive]

Finish Cancel

# Manual Integration Available in Chromatograms View

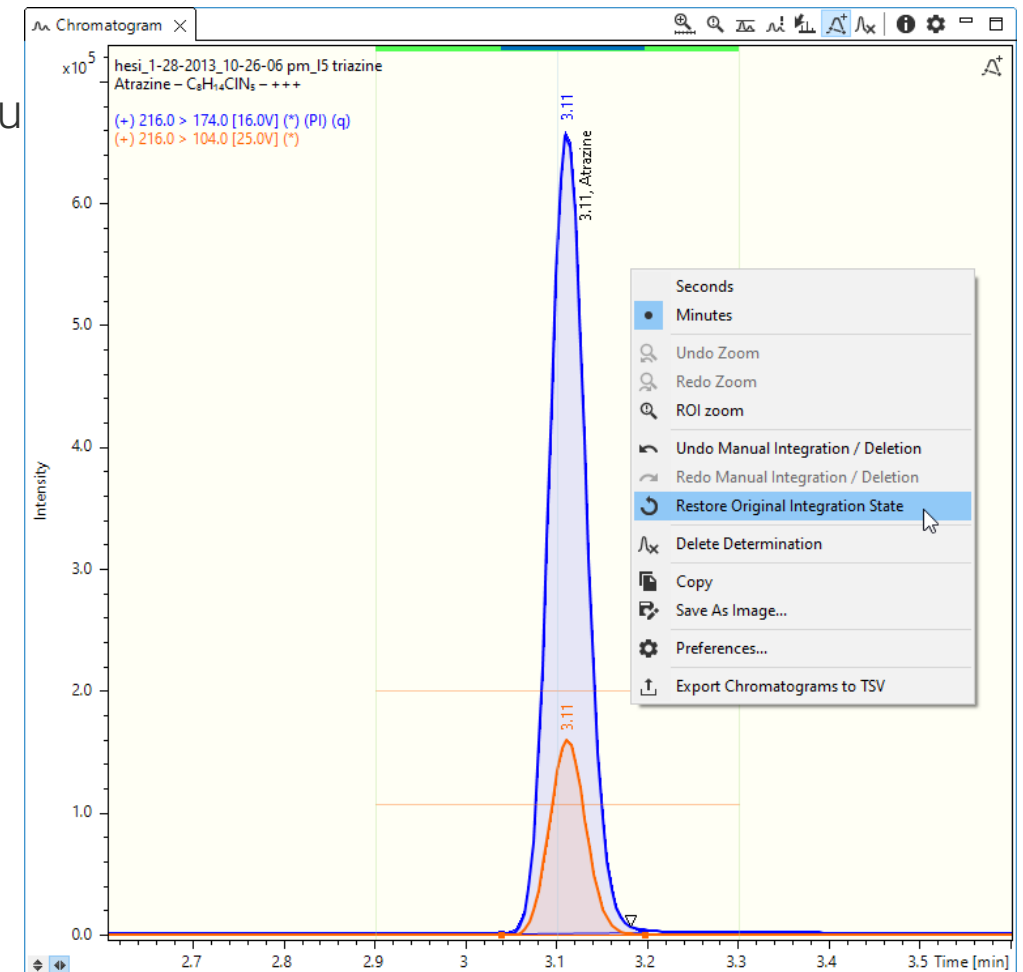
Manual integration can now be done directly in Chromatograms view



## Revert to Original Integration State

If you have done multiple manual integrations or deleted some detected peaks in chromatogram or mobilogram you can revert to the original state after processing using the command „Restore Original Integration State“ for the selected determination.

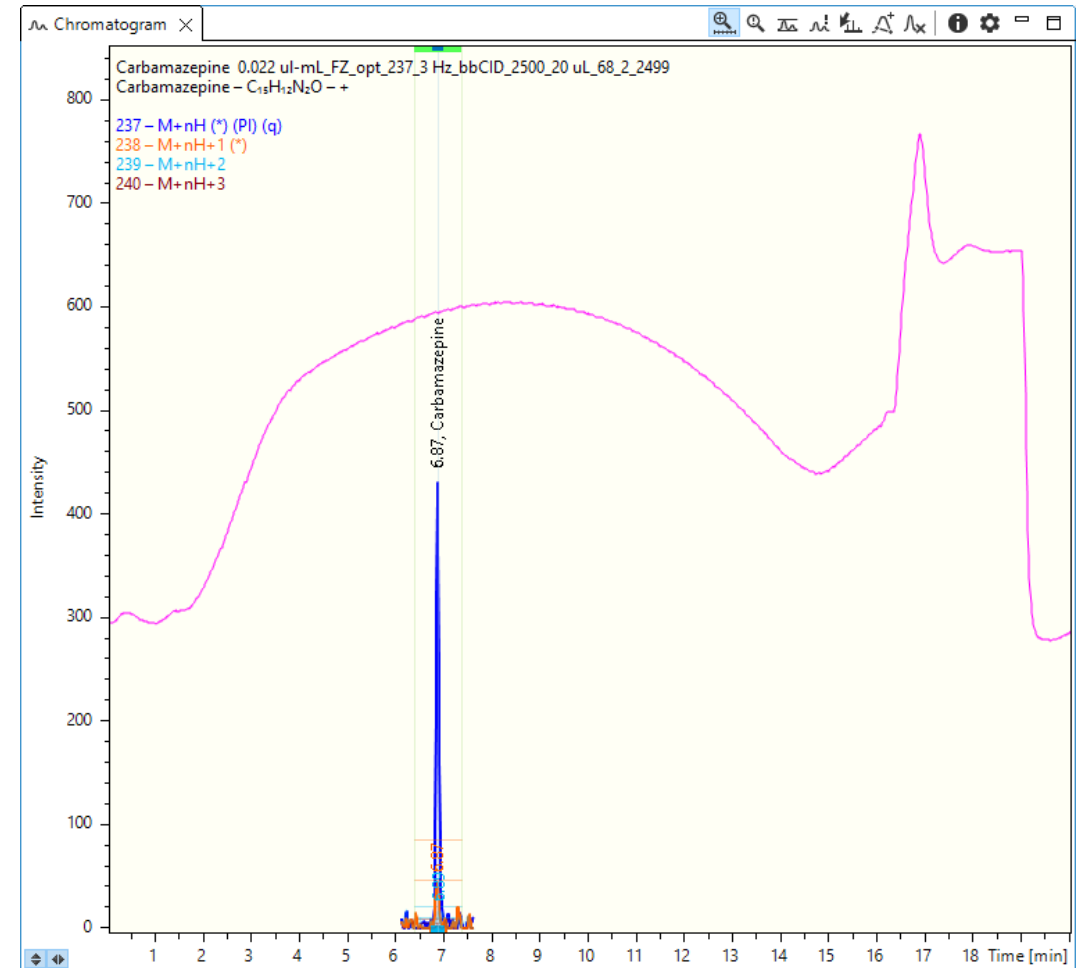
**Note:** This action can't be undone. You have to work out all required manual integration if necessary.



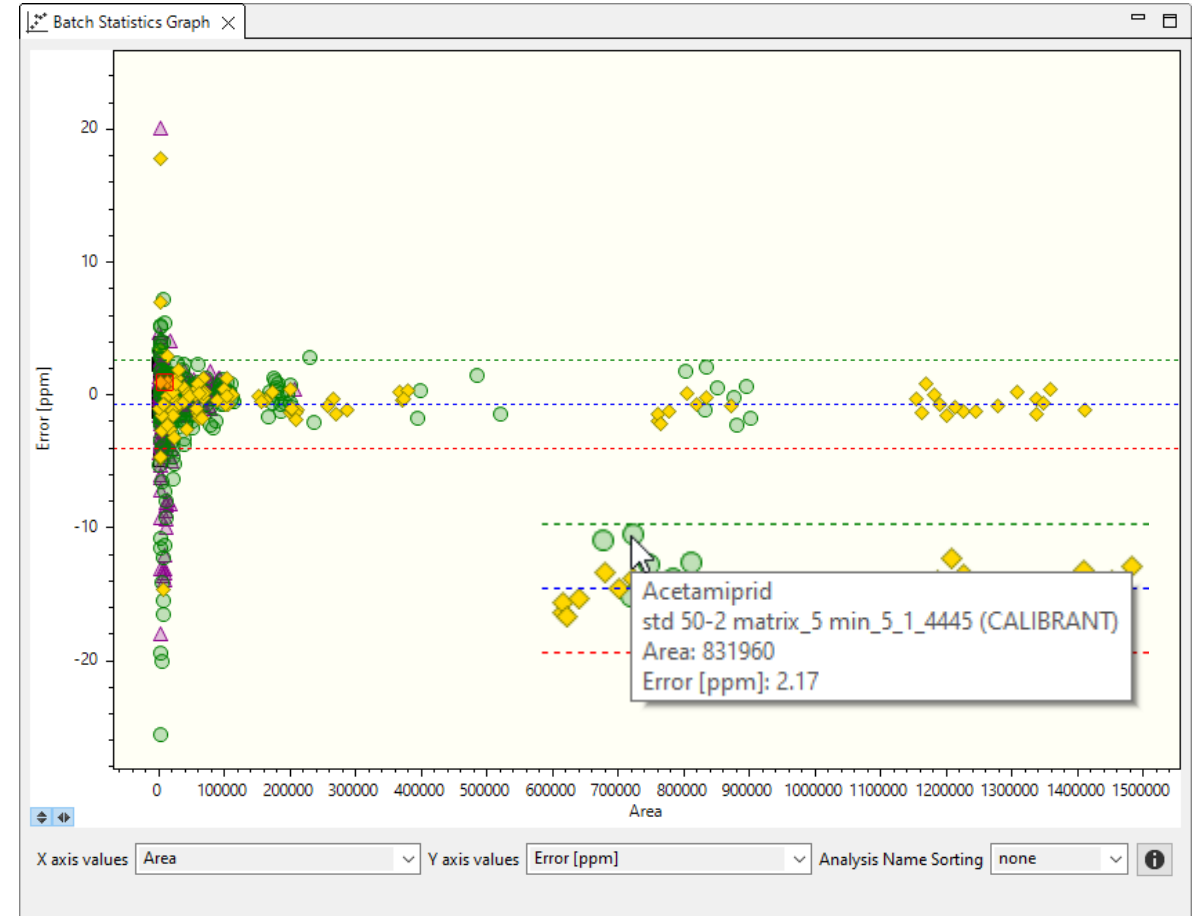
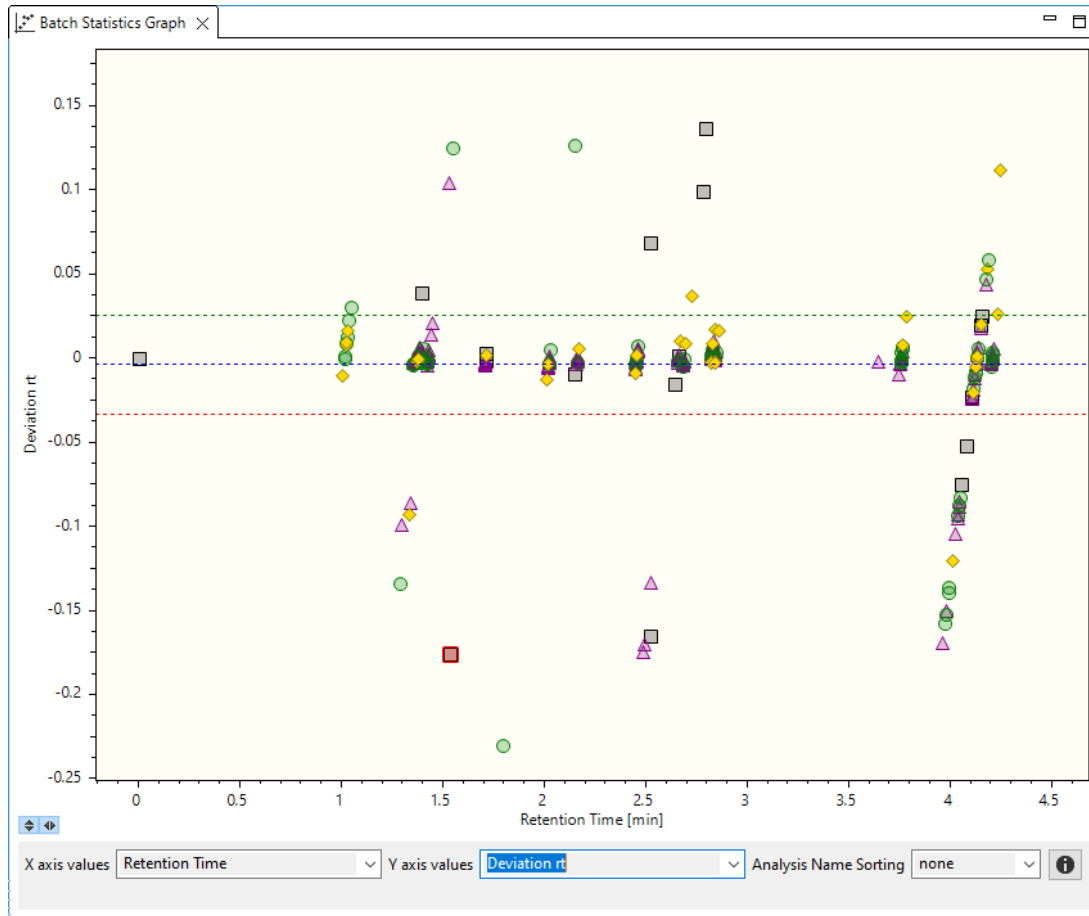
# Overlay LC-Pressure Curve in Chromatogram View

The LC pressure curve can be overlaid in the chromatogram view.

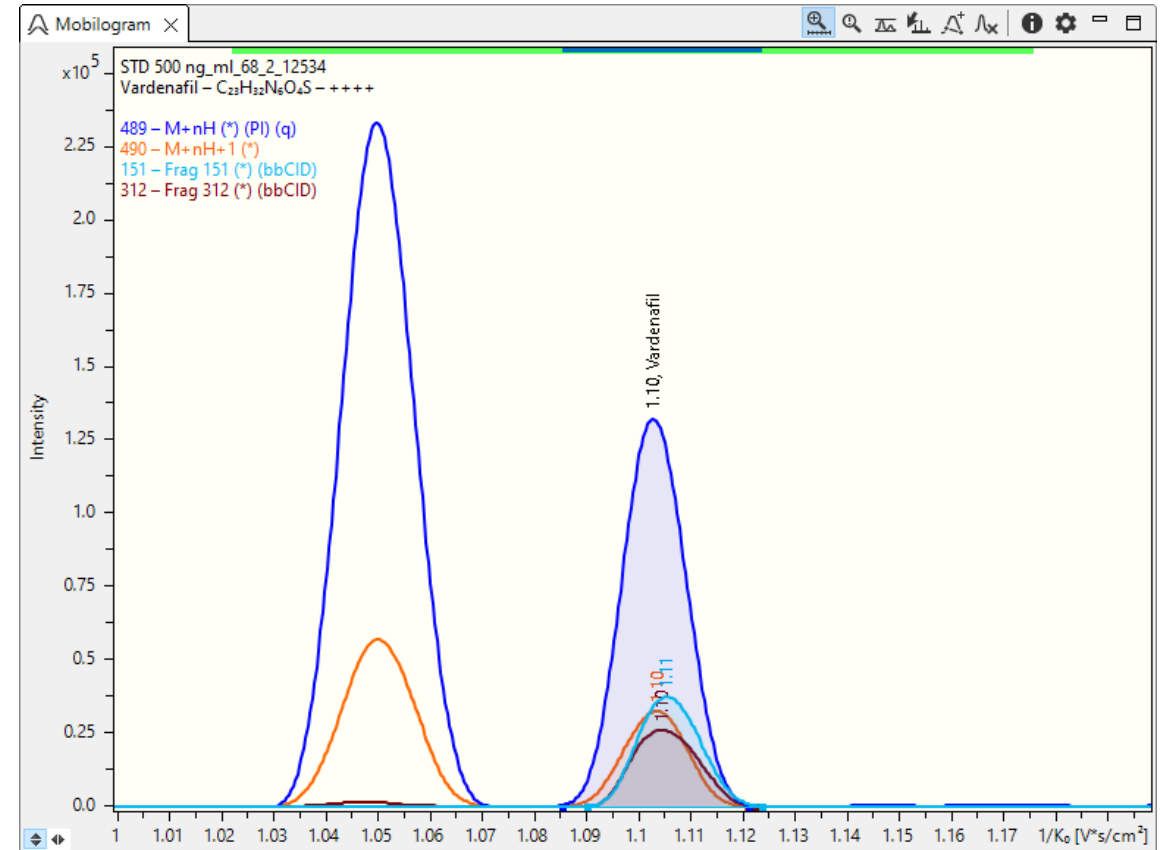
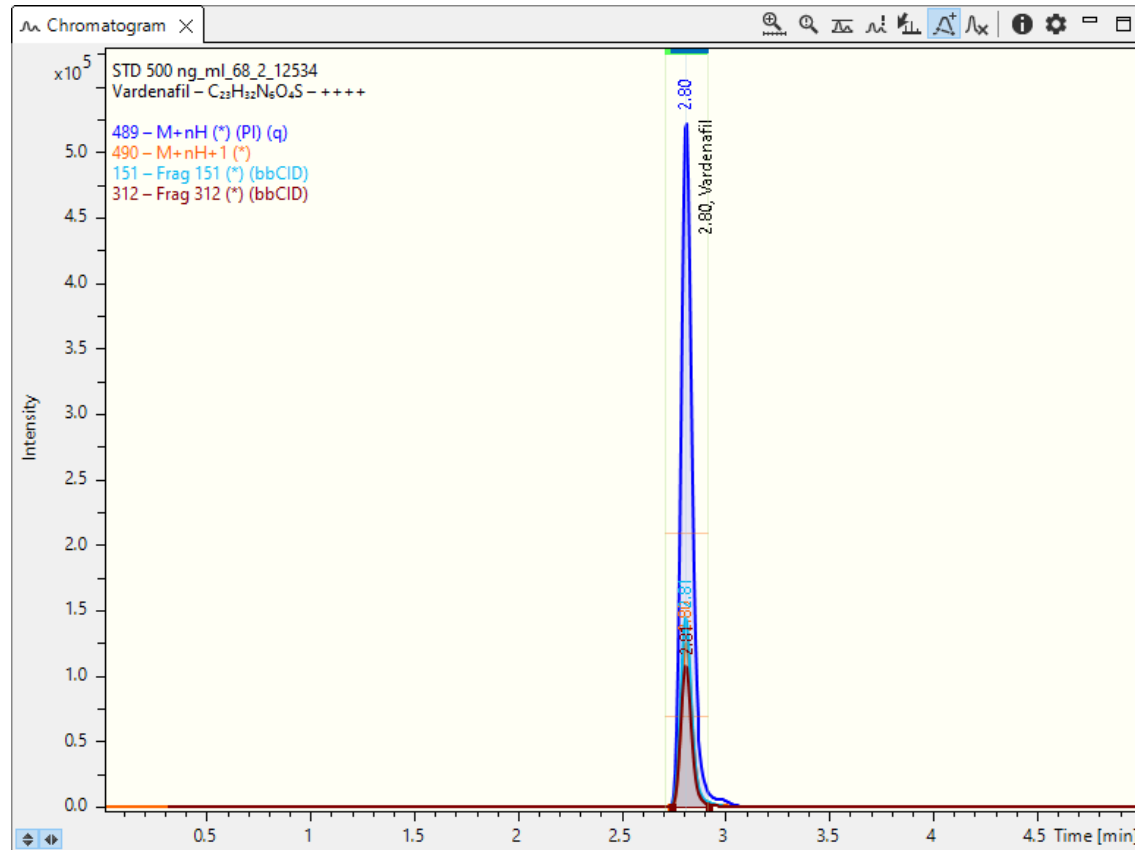
**Note:** The pressure values are normalized to 1000 and bound to the same y-axis as the MS traces.



# Show All Determinations of Selected Batch in Batch Statistics Graph



# Cleaner Toolbar for Chromatogram and Mobilogram View



Only relevant buttons remained for the most relevant actions

To add or change the displayed content open the preferences dialog 



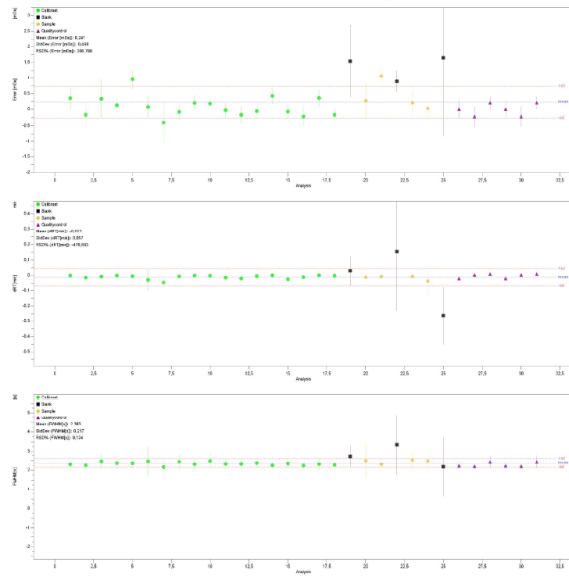
# New Report Layout Real Time QC Summary

## Demo Data Quantitation-AuditTrail – RealTimeQC Summary Report



Operator: bdal@de  
 Instrument Name: impact HDII  
 Station Name: WSBRE01-HCGB5N3  
 Instrument SN: 1825153,10011  
 TASQ Method: Demo Data Quant (5)

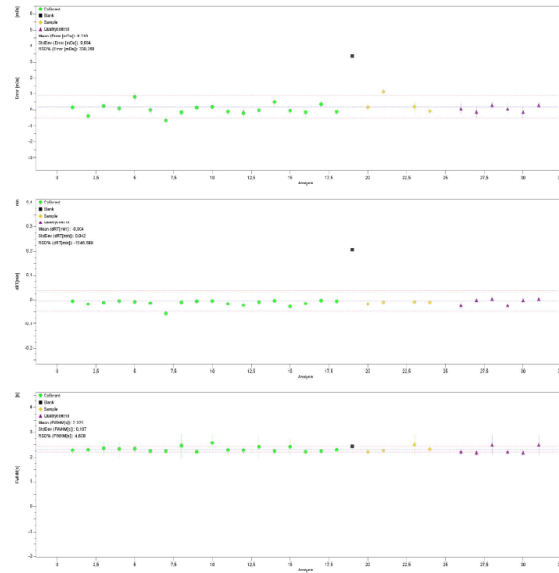
### Total Ion Count - All Analytes



## Demo Data Quantitation-AuditTrail – RealTimeQC Summary Report



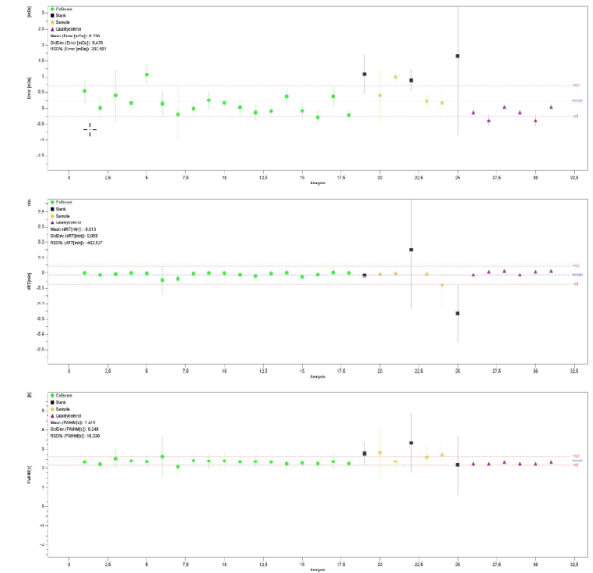
### Internal Standards only



## Demo Data Quantitation-AuditTrail – RealTimeQC Summary Report



### Analytes only

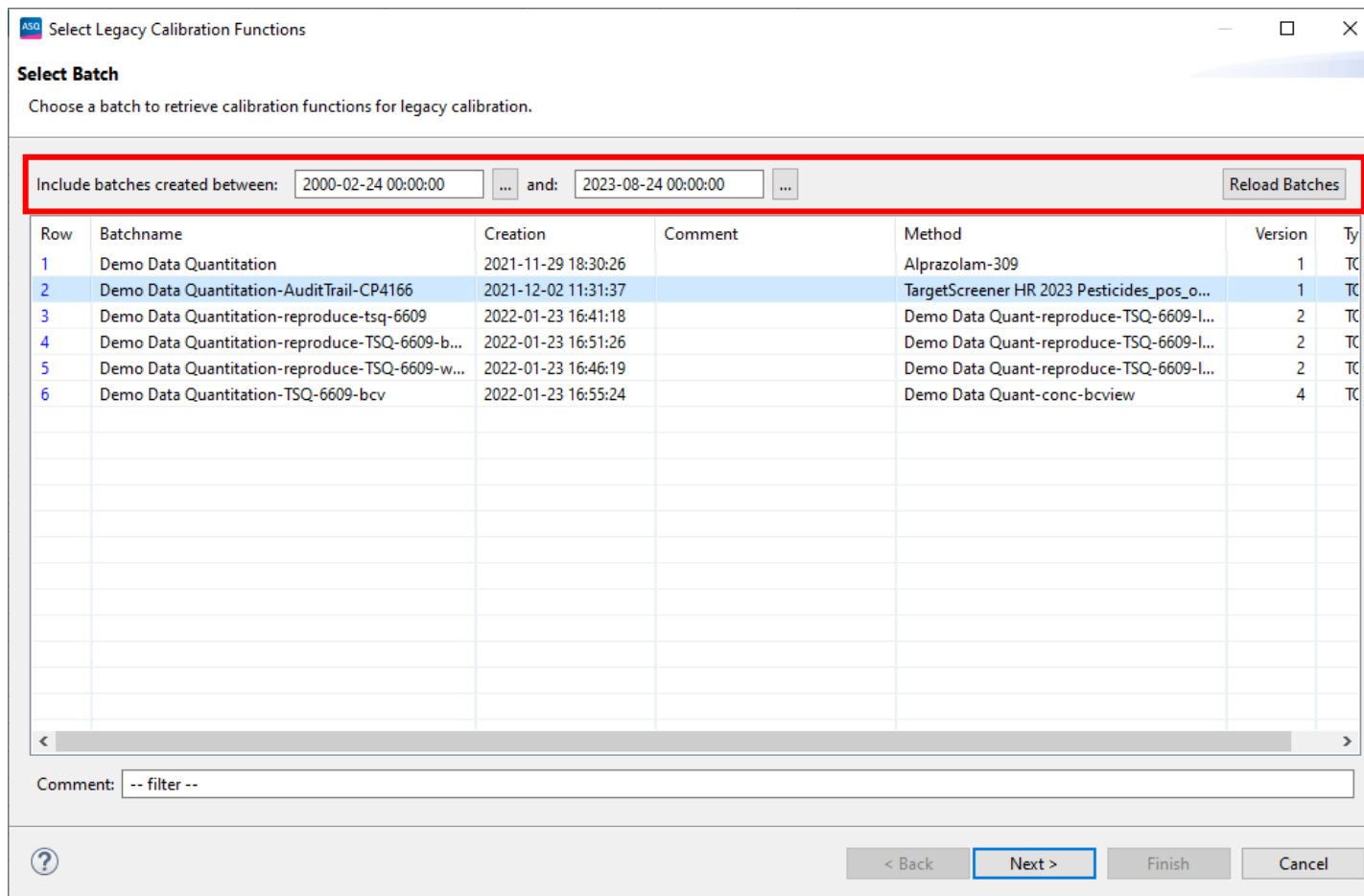


## Fix For Selecting Batches To Be Used for Legacy Calibration

If there are more than thousand batches available the assignment of calibration functions to a method to be used for legacy calibration may not offer the most recent batches in previous versions

To make sure that most recent batches are selectable an option has been added to filter batches by creation time range

If the expected batch is not shown narrow down the creation time range



Select Legacy Calibration Functions

Select Batch

Choose a batch to retrieve calibration functions for legacy calibration.

Include batches created between: 2000-02-24 00:00:00 ... and: 2023-08-24 00:00:00 ... Reload Batches

Row	Batchname	Creation	Comment	Method	Version	Typ
1	Demo Data Quantitation	2021-11-29 18:30:26		Alprazolam-309	1	TC
2	Demo Data Quantitation-AuditTrail-CP4166	2021-12-02 11:31:37		TargetScreener HR 2023 Pesticides_pos_o...	1	TC
3	Demo Data Quantitation-reproduce-tsq-6609	2022-01-23 16:41:18		Demo Data Quant-reproduce-TSQ-6609-I...	2	TC
4	Demo Data Quantitation-reproduce-TSQ-6609-b...	2022-01-23 16:51:26		Demo Data Quant-reproduce-TSQ-6609-I...	2	TC
5	Demo Data Quantitation-reproduce-TSQ-6609-w...	2022-01-23 16:46:19		Demo Data Quant-reproduce-TSQ-6609-I...	2	TC
6	Demo Data Quantitation-TSQ-6609-bcv	2022-01-23 16:55:24		Demo Data Quant-conc-bcview	4	TC

Comment: -- filter --

< Back Next > Finish Cancel



# The New Compass Platform 8.0 Introduces Secure Communication

Client and server can communicate now using SSL encryption

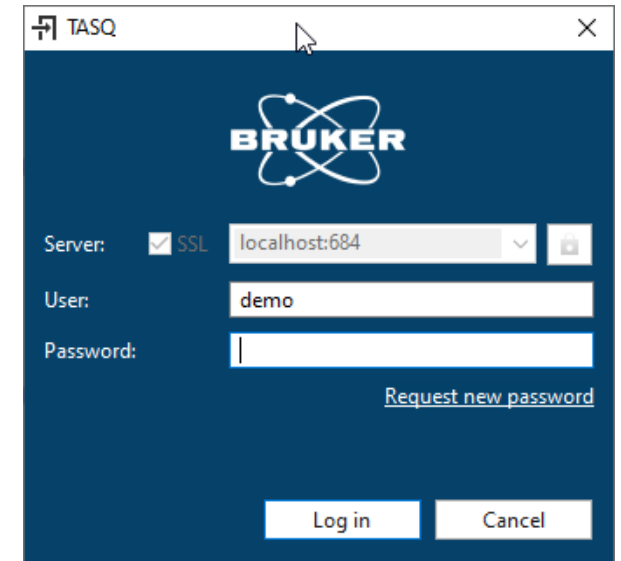
For CORBA communication port 684 is used

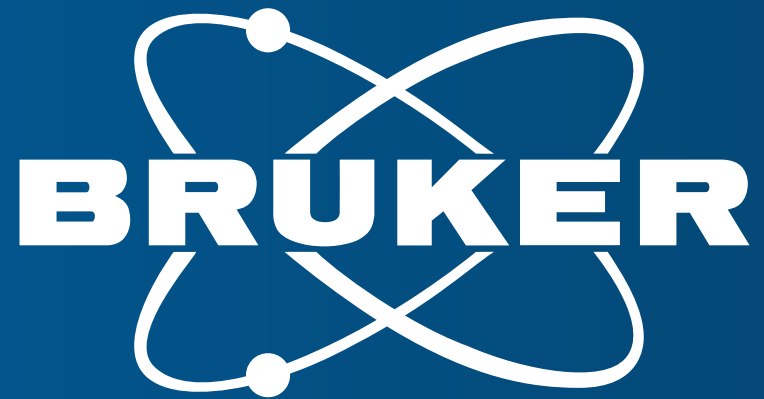
For HTTPS communication port 443 is used

The logon dialog now offers to switch SSL communication off or on

**Note:** If you are upgrading you have to run the Compass Server Selector again to configure the two new ports

**Note:** You may have to update the firewall settings for incoming and outgoing network communication to allow to use port 443 and 684





Innovation with Integrity