23.0331

Clarity™

ADVANCED CHROMATOGRAPHY SOFTWARE

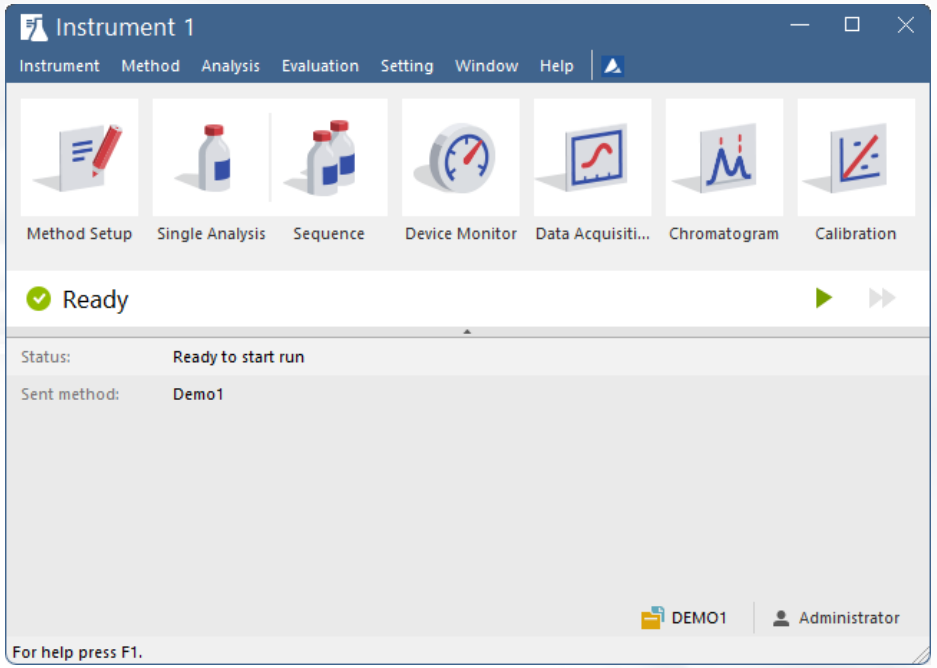
CLARITY TRAINING

ADVANCED – PART 2

DataApex

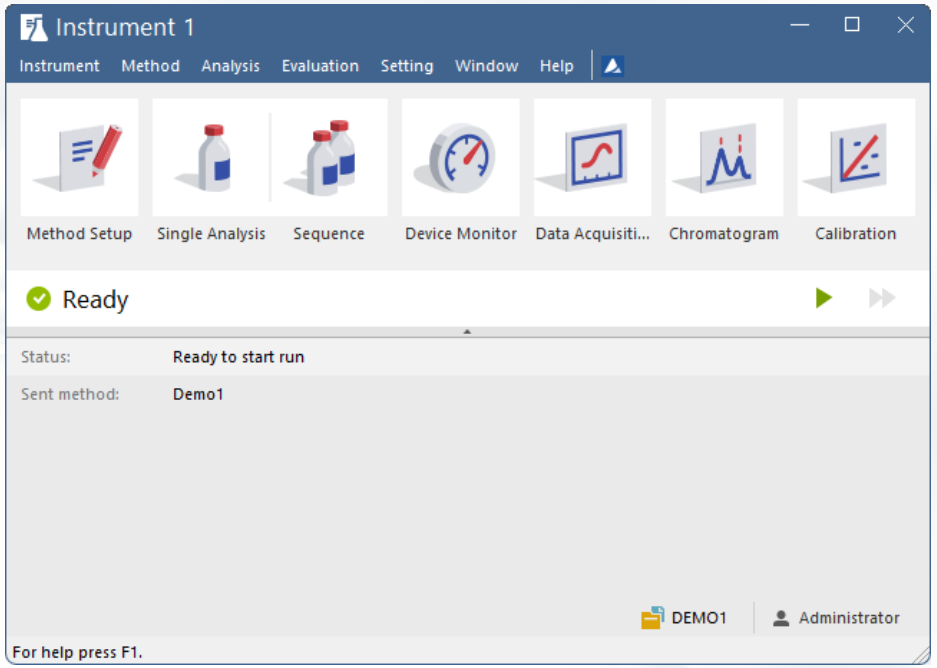
AGENDA

- Chromatogram window
  - Column setup, User columns, Noise & Drift
  - Mathematical operations, Labels
  - Result table, User variables
  - Summary table, Performance table
  - Force peak name, Peak coloring, Graph properties
- Calibration
  - LOD, LOQ
  - Calibration Options, Manual Calibration
  - Details of Calibration Point
  - Bracketing and Standard Addition
- Calculations
  - ISTD, Normalized %
- Groups



AGENDA

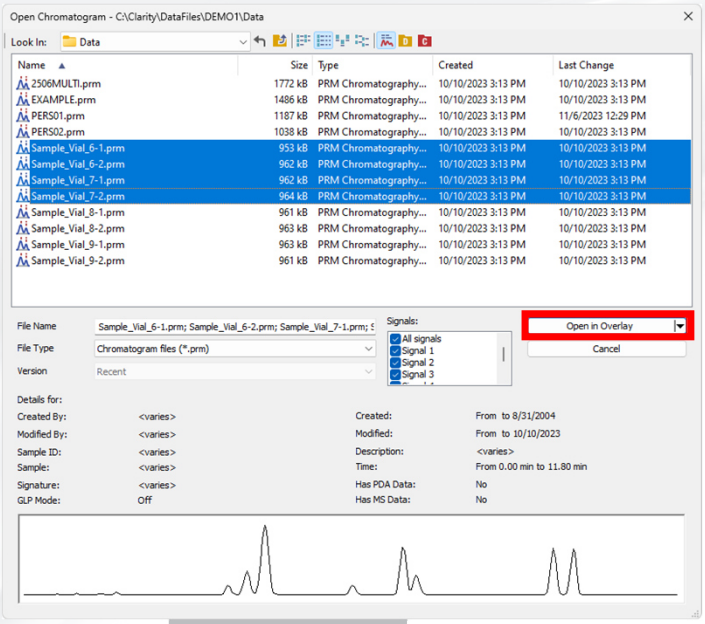
- Chromatogram window
  - Column setup, User columns, Noise & Drift
  - Mathematical operations, Labels
  - Result table, User variables
  - Summary table, Performance table
  - Force peak name, Peak coloring, Graph properties
- Calibration
  - LOD, LOQ
  - Calibration Options, Manual Calibration
  - Details of Calibration Point
  - Bracketing and Standard Addition
- Calculations
  - ISTD, Normalized %
- Groups

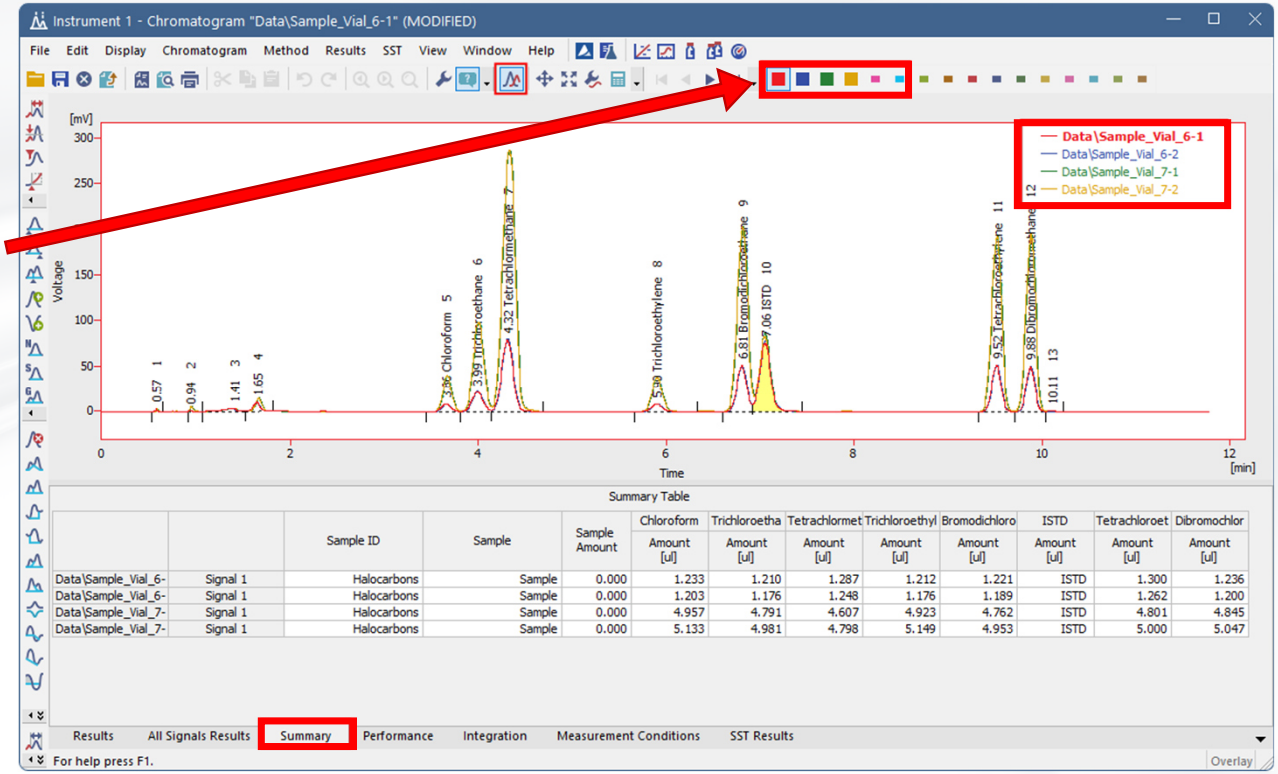


CHROMATOGRAM WINDOW

OVERLAY

- Comparing multiple chromatograms
  - Max. number is set in User Options
- Summary table shows results of the displayed chromatograms/signals
- Hide/show signals via Ctrl+Click on signal color

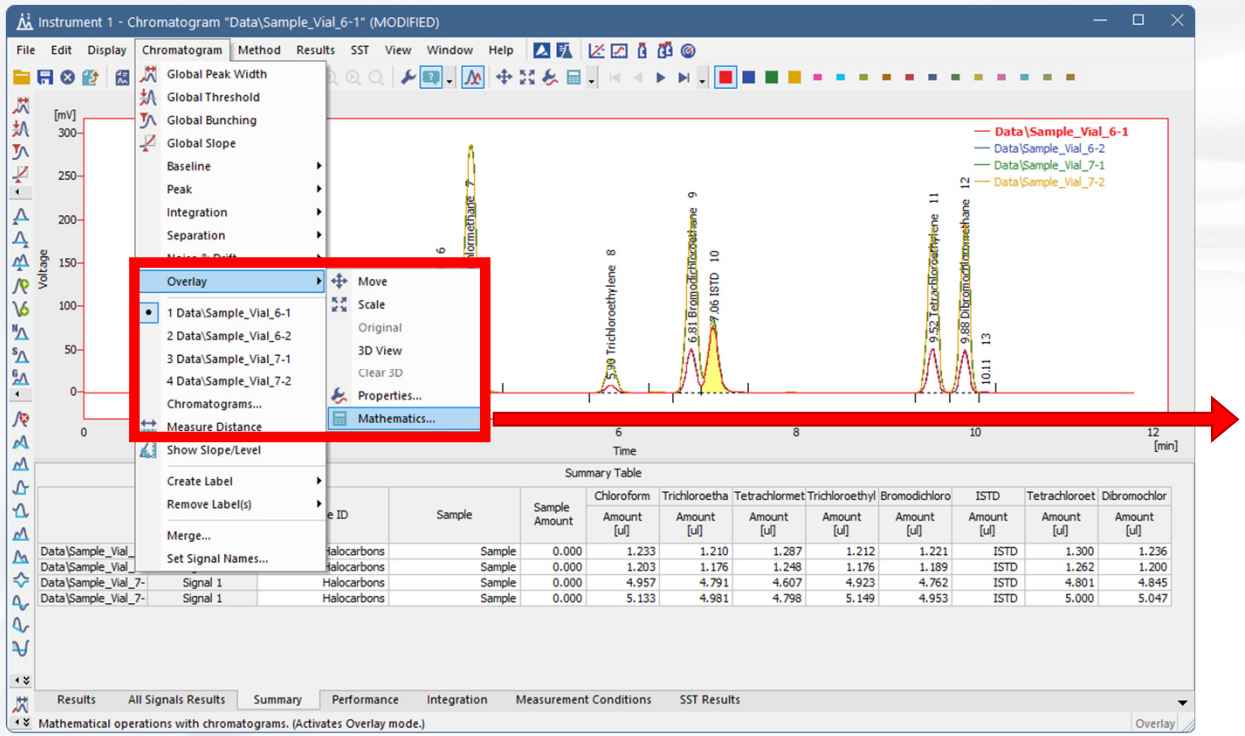


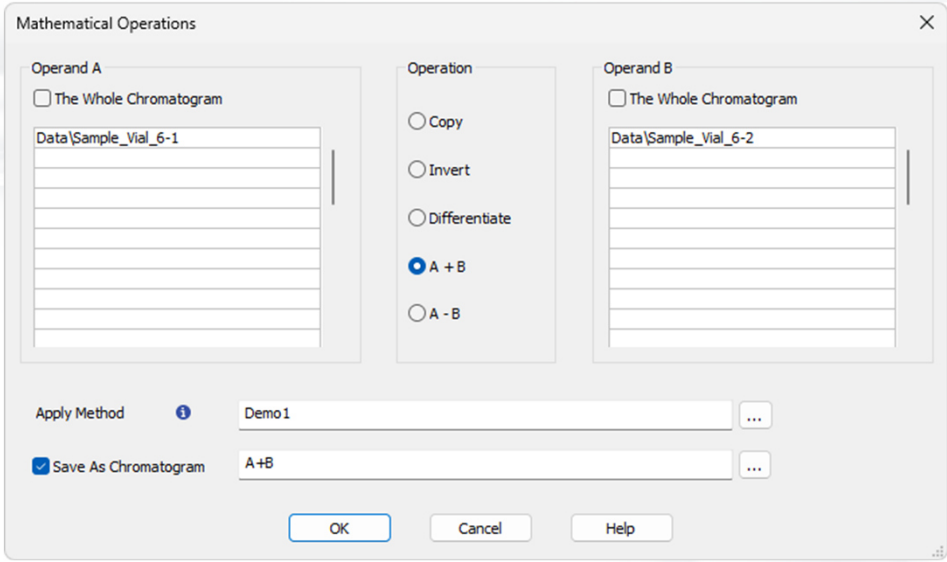


CHROMATOGRAM WINDOW

MATHEMATICAL OPERATIONS

- Mathematical operations between signals/chromatograms

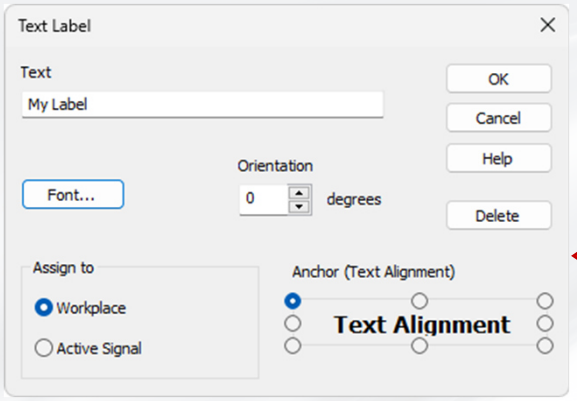


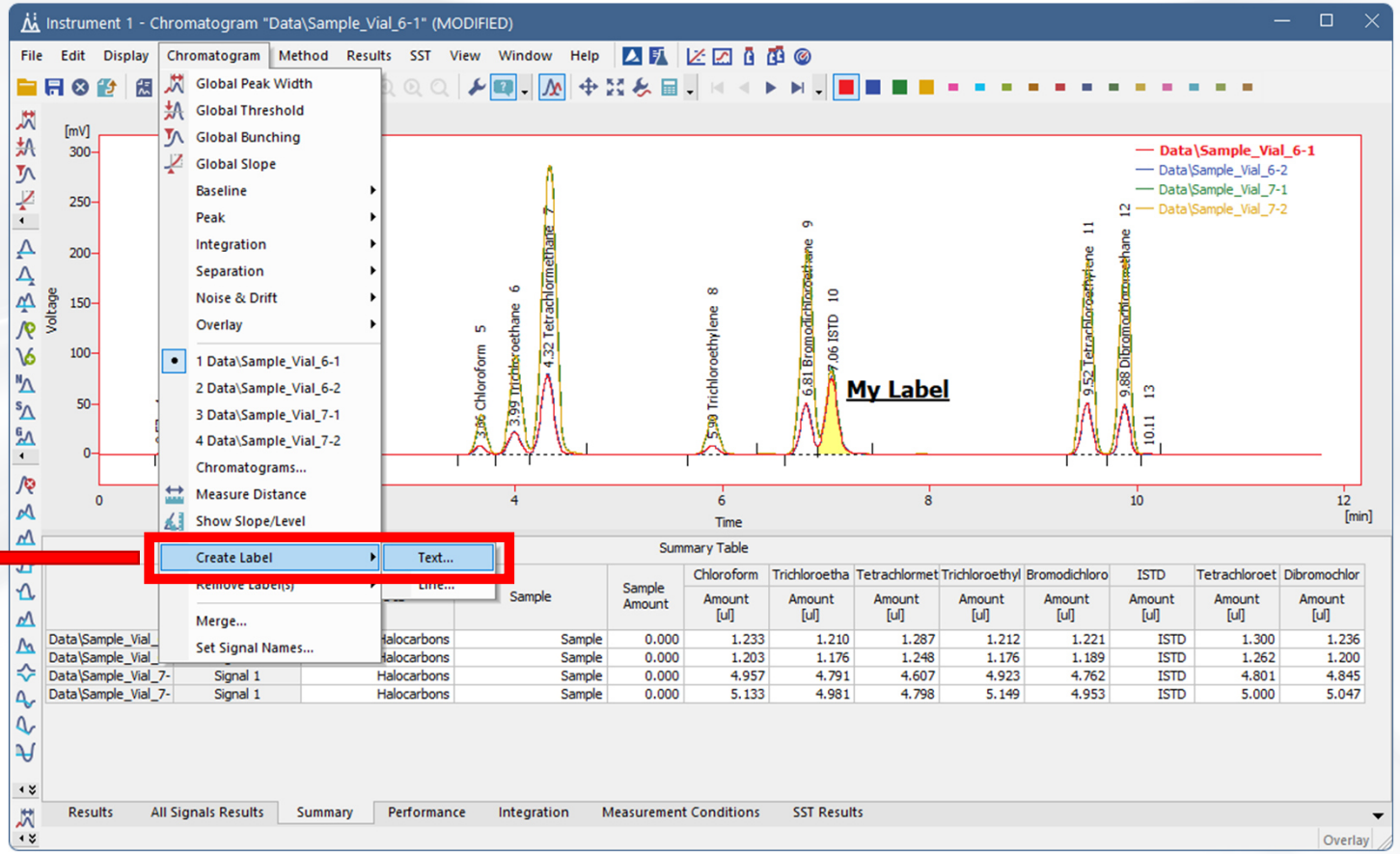


CHROMATOGRAM WINDOW

LABELS

- Add text labels or lines

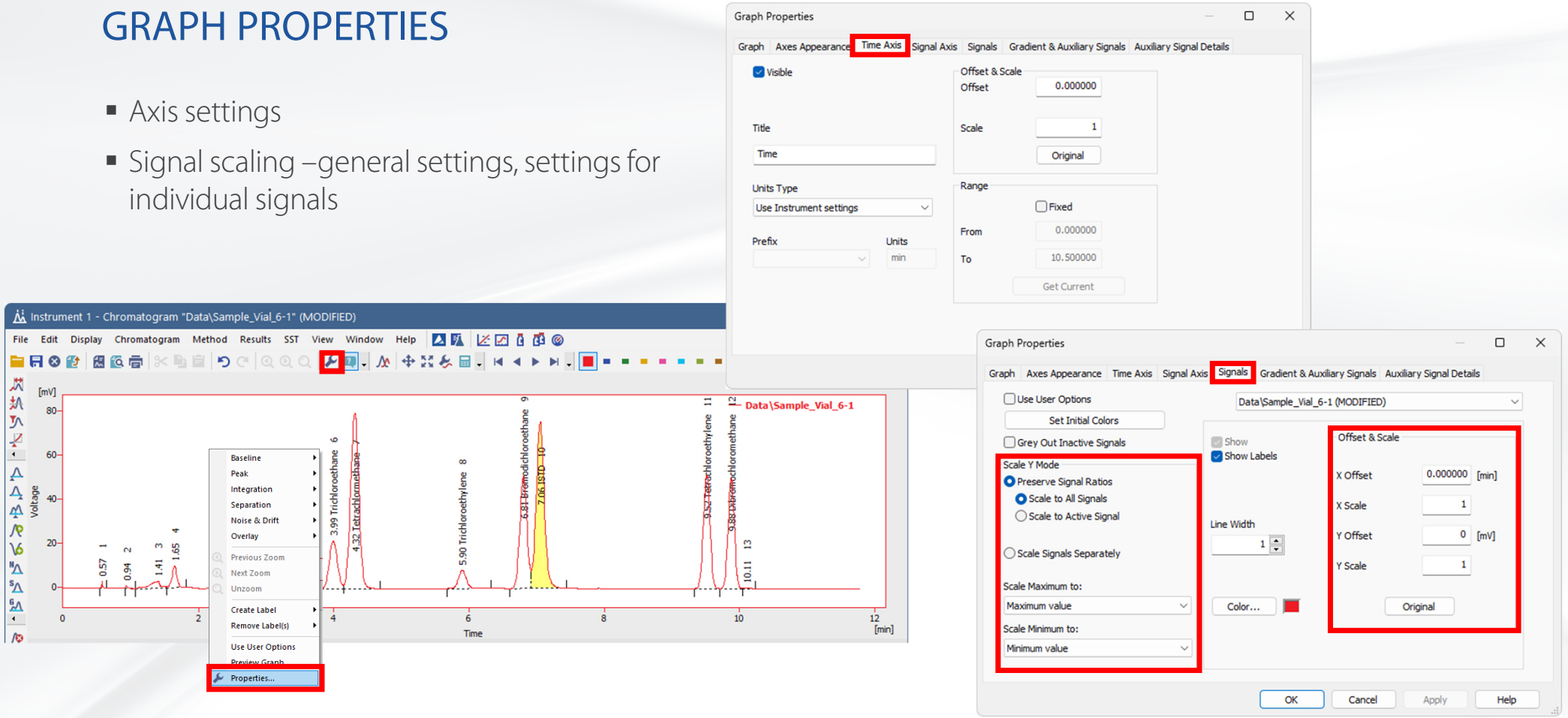




CHROMATOGRAM WINDOW

GRAPH PROPERTIES

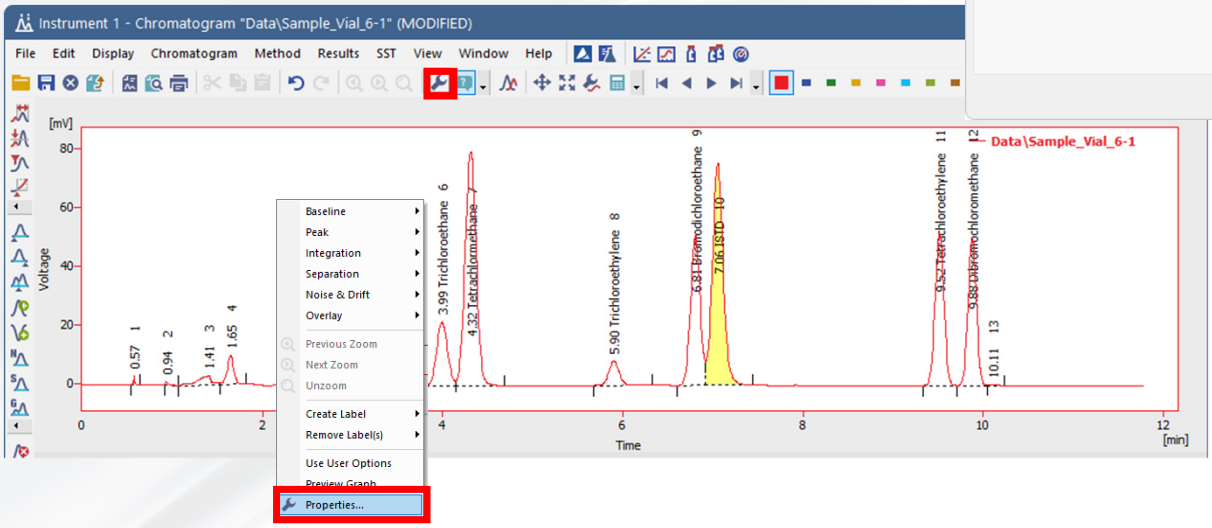
- Axis settings
- Signal scaling –general settings, settings for individual signals

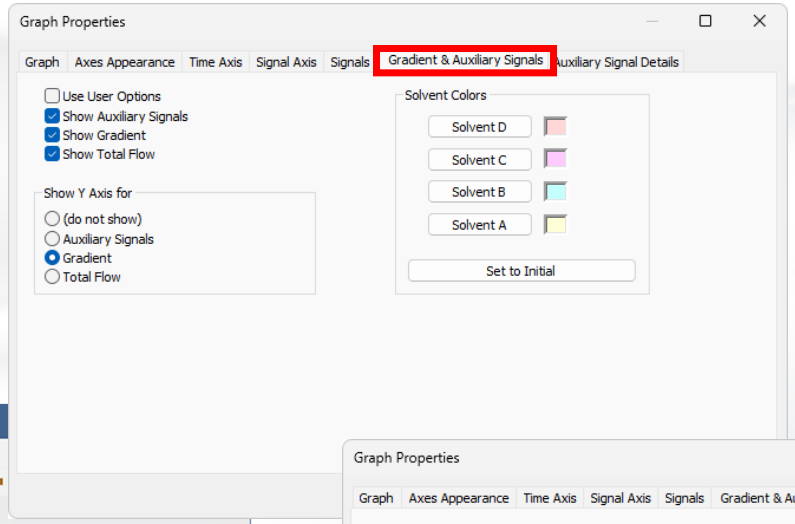


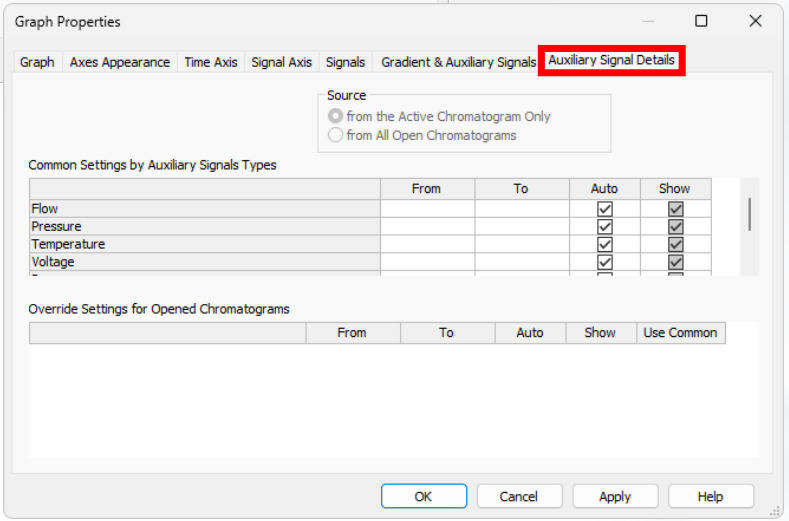
CHROMATOGRAM WINDOW

GRAPH PROPERTIES

- Gradient display option
- Auxiliary signals options



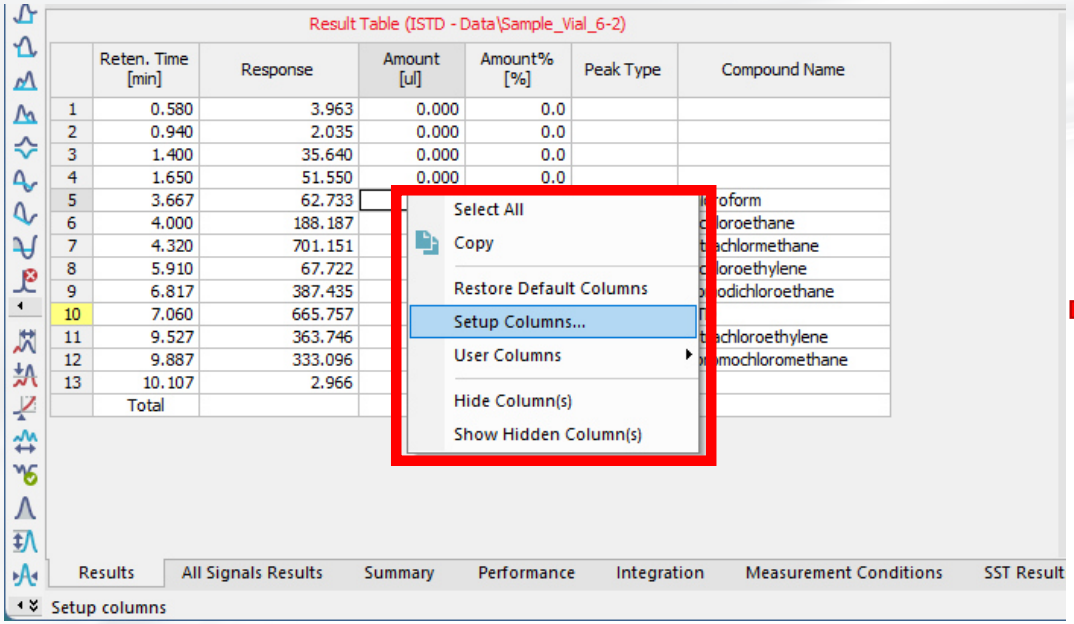


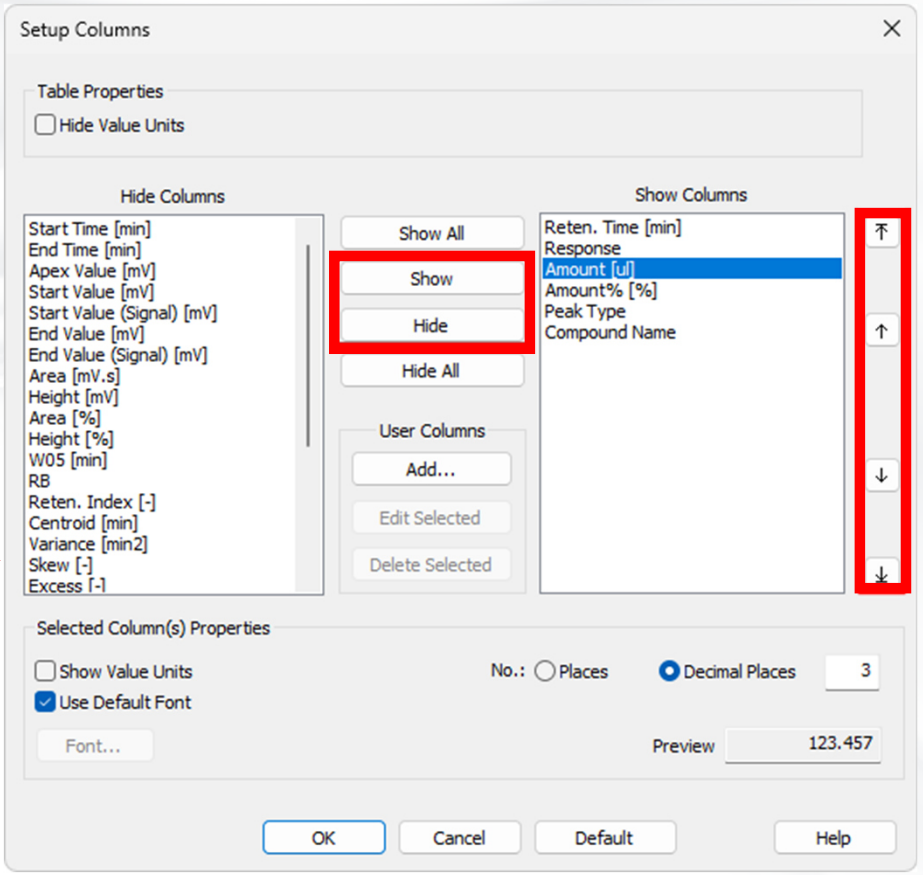


CHROMATOGRAM WINDOW

SETUP COLUMNS

- Operable from the context menu of any table
- Hide/Show columns
- Change the order of columns

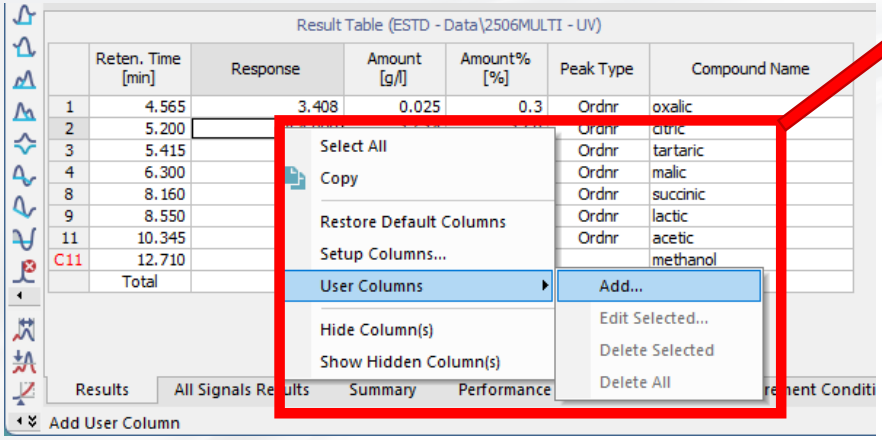


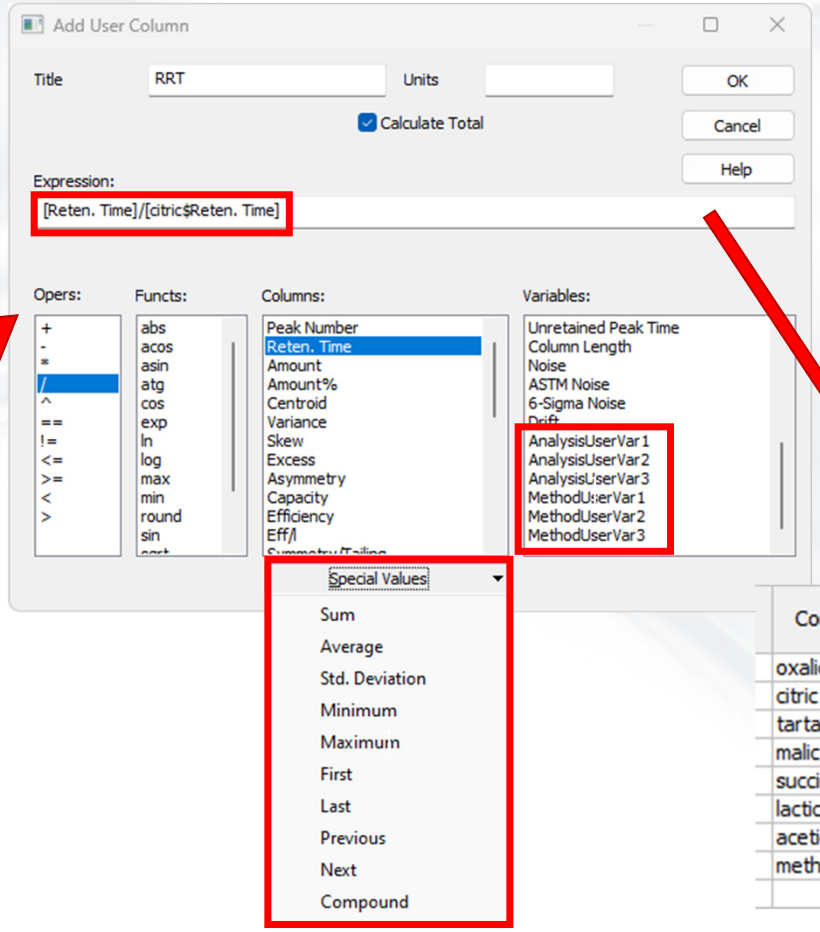


CHROMATOGRAM WINDOW

USER COLUMNS – RRT (RELATIVE RETENTION TIME)

- Access via context menu in Result/Summary table
- Add custom calculations
- Special values menu for more options
- Specify user variables



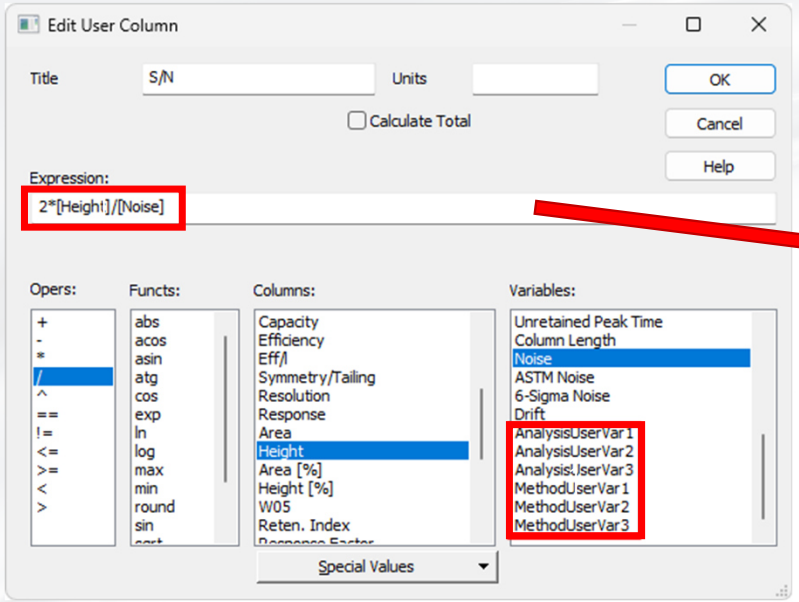


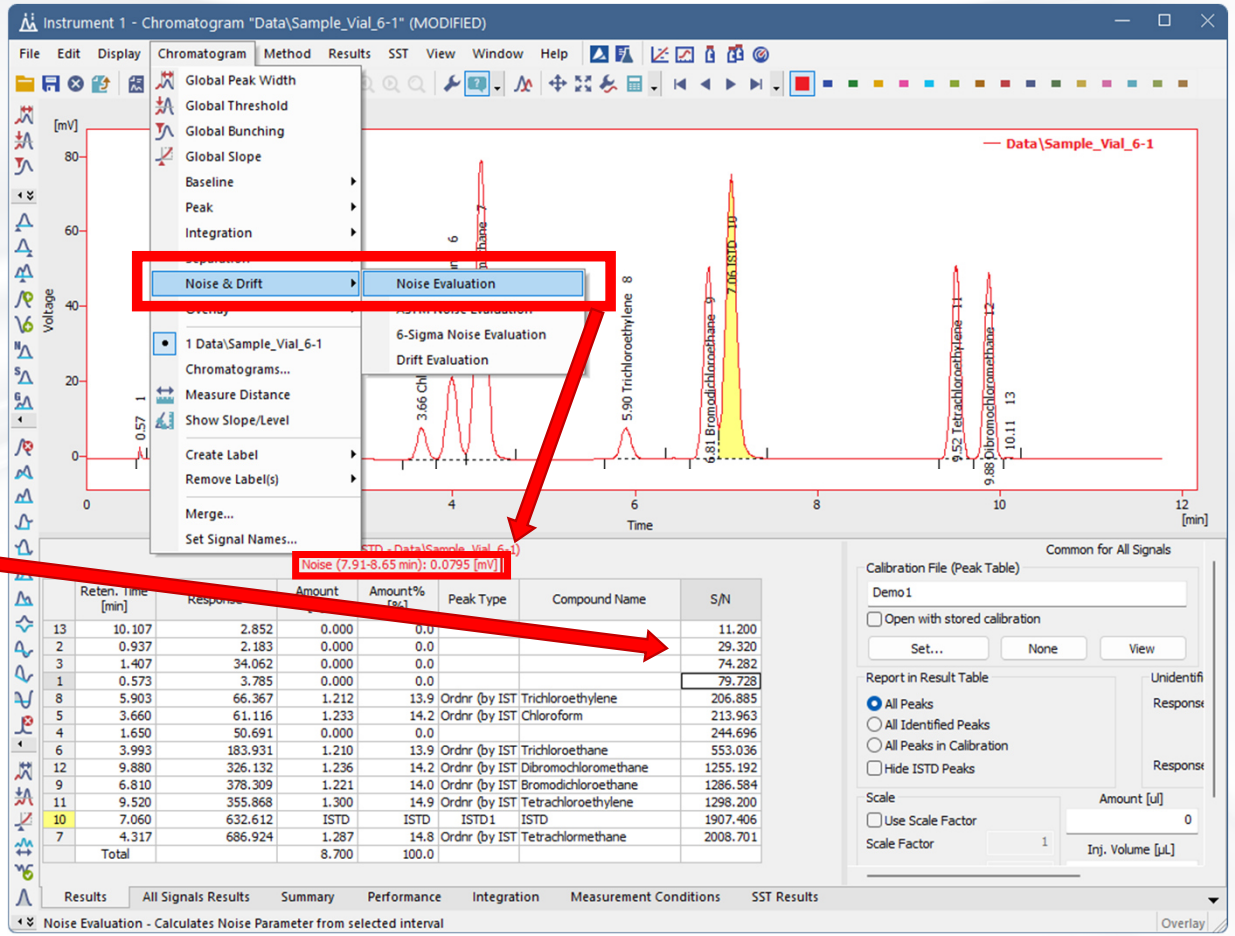
Compound Name	RRT
oxalic	0.878
citric	1.000
tartaric	1.041
malic	1.212
succinic	1.569
lactic	1.644
acetic	1.989
methanol	2.444
	11.778

CHROMATOGRAM WINDOW

USER COLUMNS – NOISE & DRIFT

- Set noise interval
- Add Signal/Noise calculation to a user column
- User variables can be used





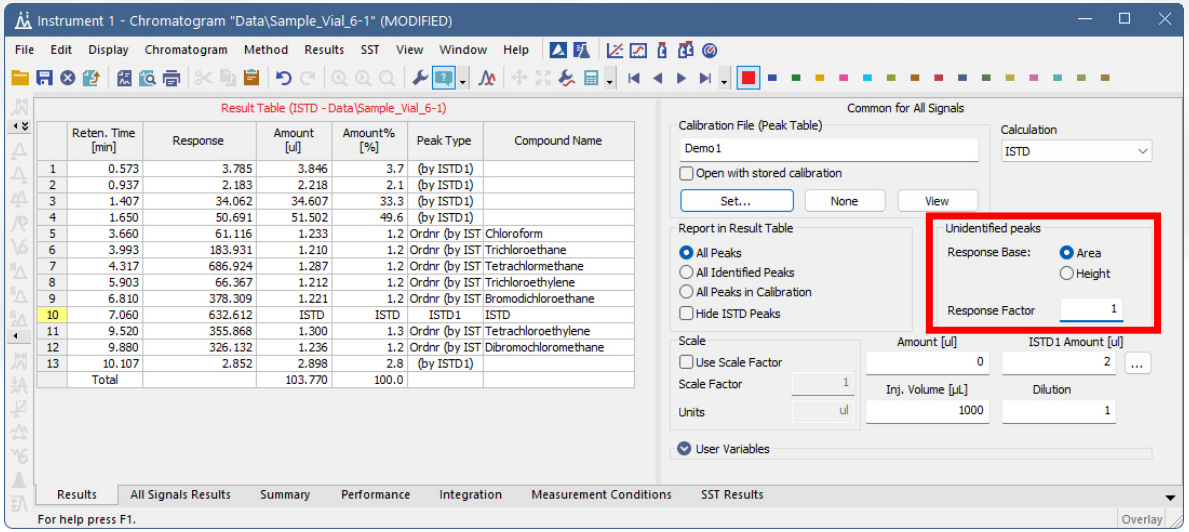
CHROMATOGRAM WINDOW

UNIDENTIFIED PEAKS – UNCALIBRATED RESPONSE

- Manually assign response base and factor to **unidentified peaks** (peaks not present in calibration)
- Calculation of amounts of unidentified (uncalibrated) compounds:

$$\text{Amount} = [\text{Response Base}] \times [\text{Response Factor}]$$

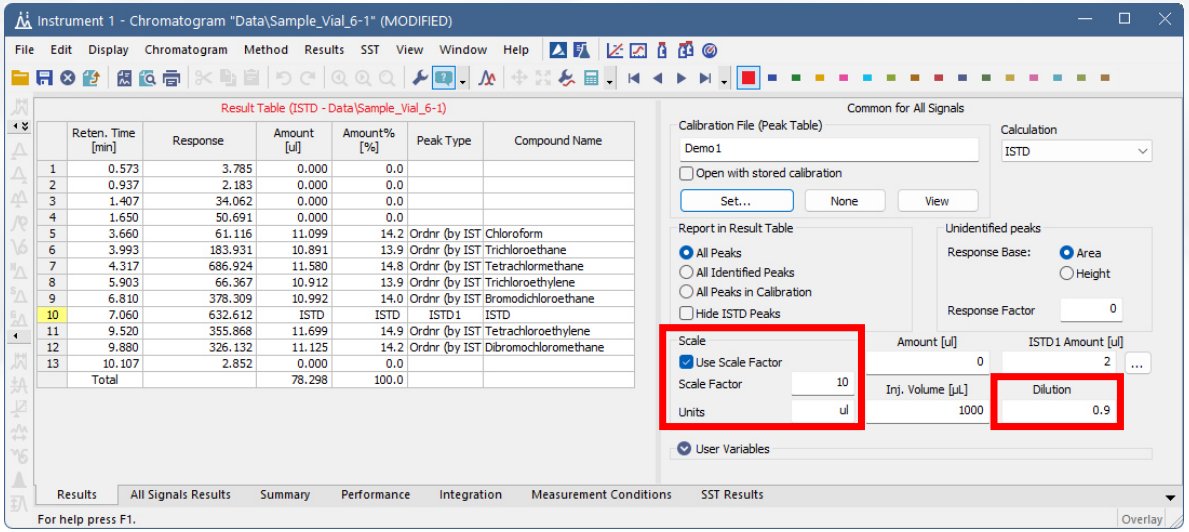
- Provides a "single-point quantification" of unidentified compounds (e.g., for universal response detectors like ELSD, FID, RI, etc.)



CHROMATOGRAM WINDOW

SCALE & DILUTION

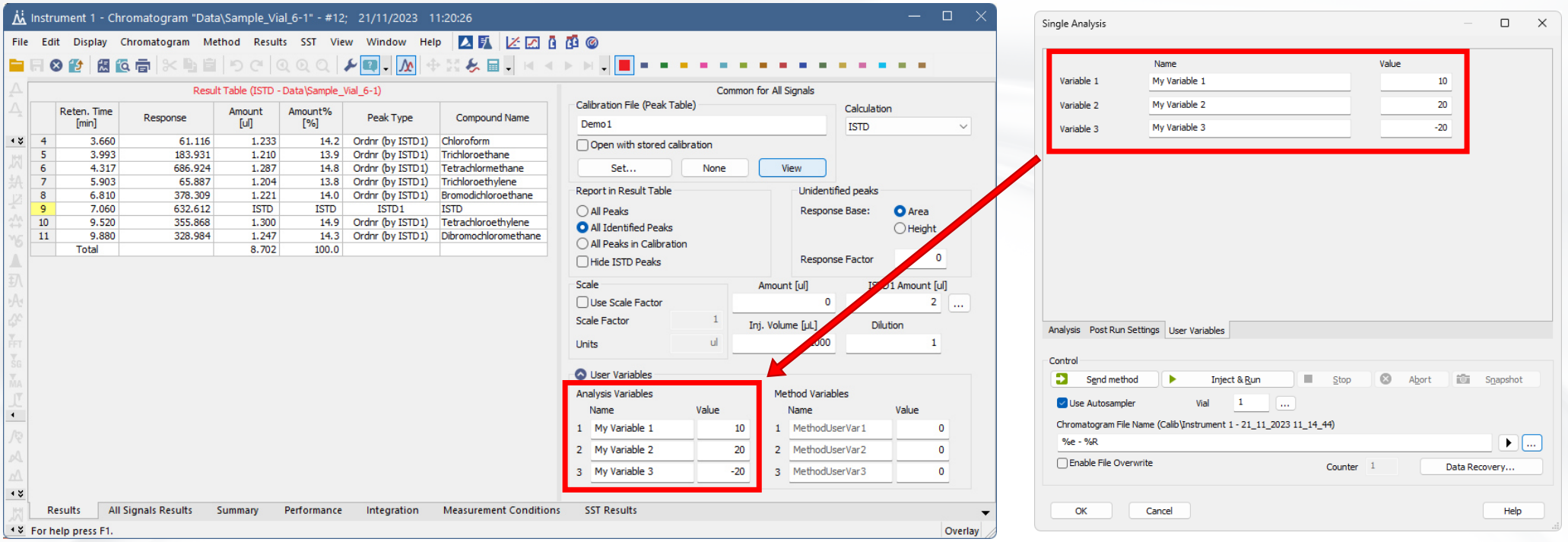
- **Scale** factor multiplies values in the Amount column and the Sample Amount (the entered units are used in the Amount when scaled, overriding the calibration settings)
  - Method-specific (can be used only when calibration is set)
- **Dilution** multiplies values in the Amount column
  - Sample-specific (can also be entered via Sequence or Single Analysis)



CHROMATOGRAM WINDOW

USER VARIABLES – ANALYSIS VARIABLES

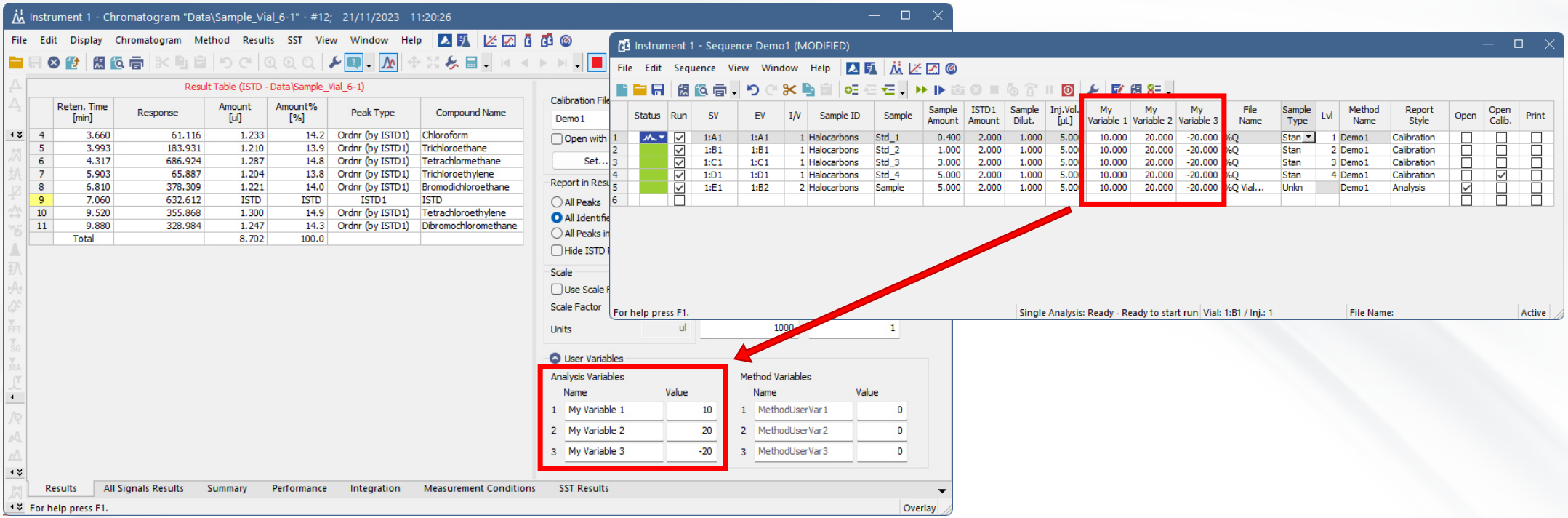
- **Analysis Variables** are propagated from **Single Analysis** or Sequence to the measured chromatogram
  - These can be used for custom calculations in the Result Table



CHROMATOGRAM WINDOW

USER VARIABLES – ANALYSIS VARIABLES

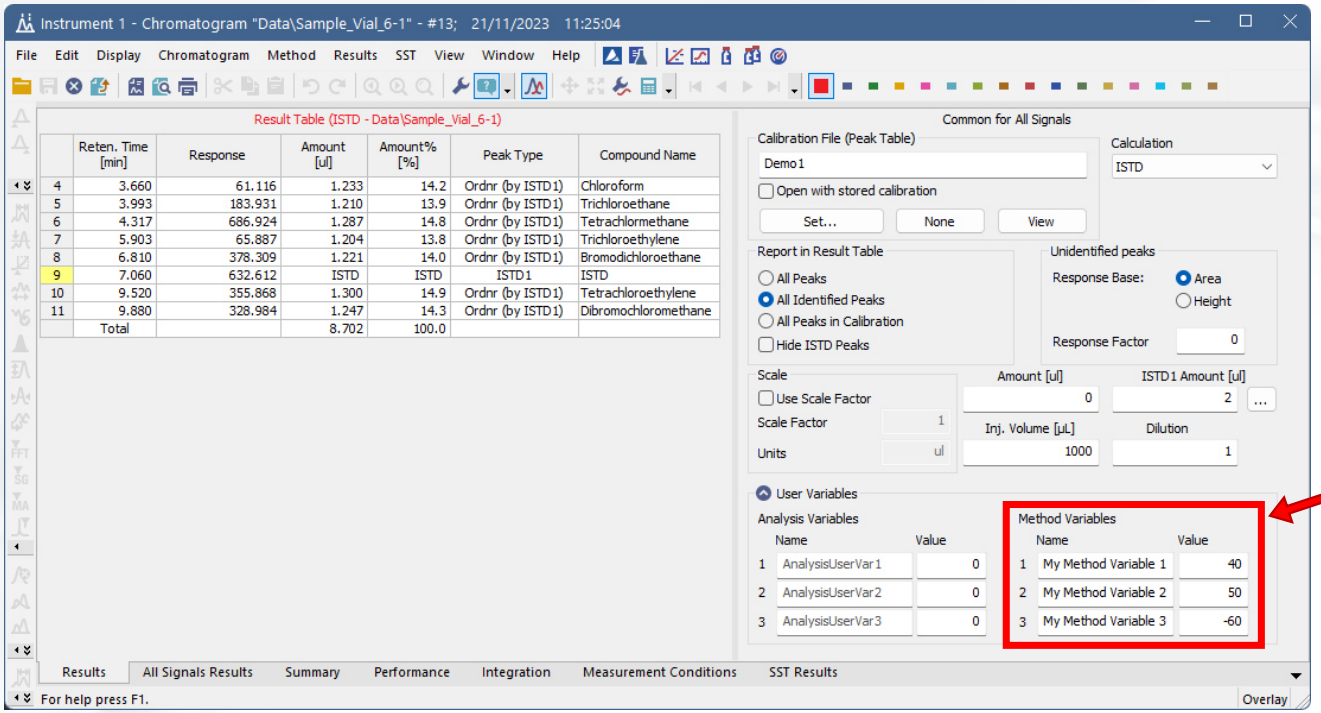
- **Analysis Variables** are propagated from Single Analysis or **Sequence** to the measured chromatogram
  - These can be used for custom calculations in the Result Table

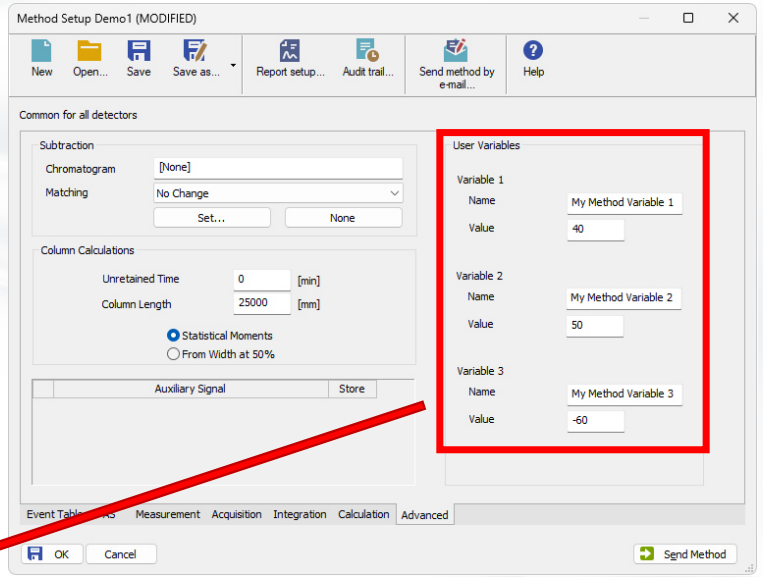


CHROMATOGRAM WINDOW

USER VARIABLES – METHOD VARIABLES

- **Method Variables** are propagated from Method Setup – Advanced tab to the measured chromatogram
  - These can be used for custom calculations in the Result Table

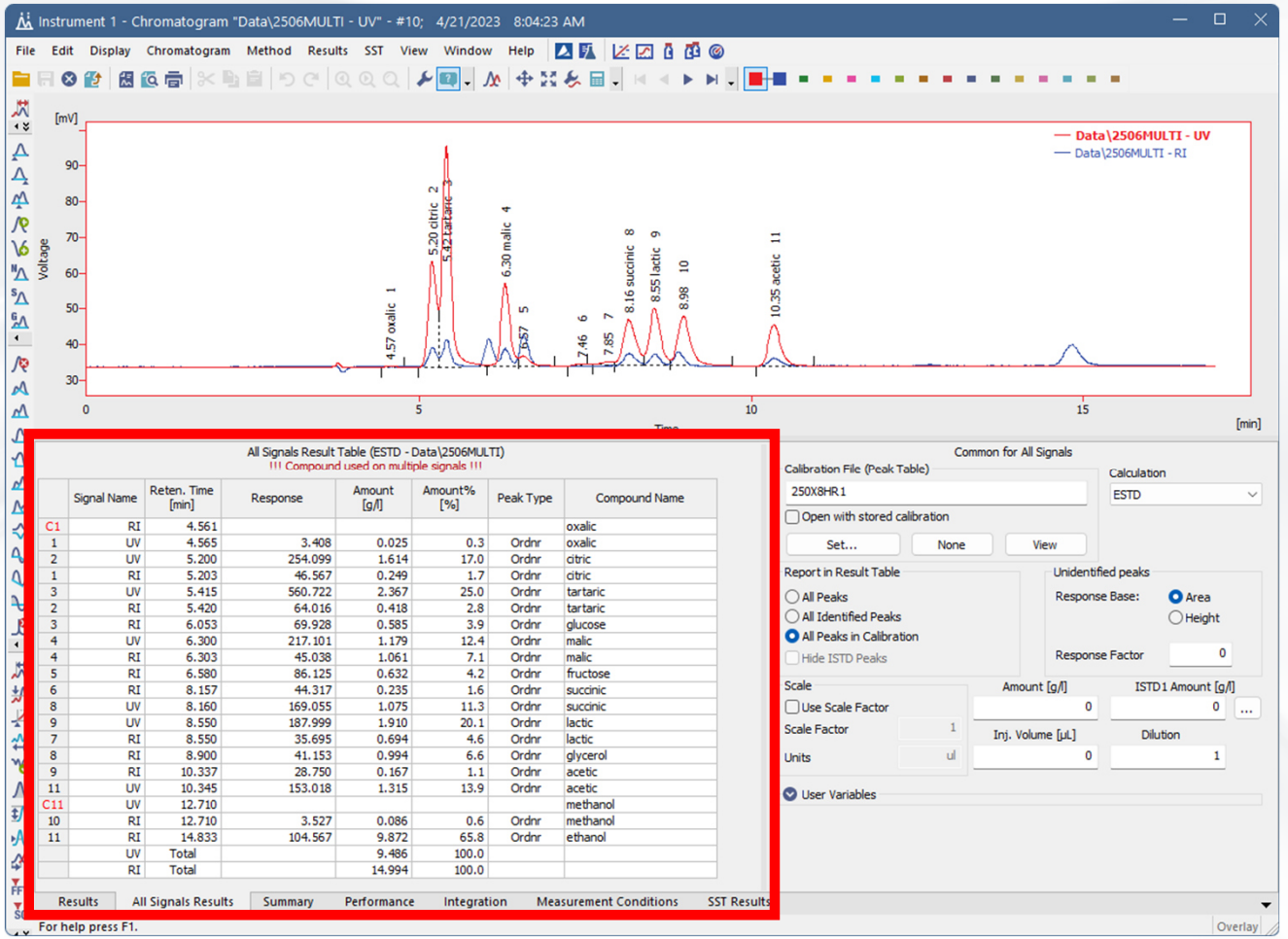




CHROMATOGRAM WINDOW

ALL SIGNALS RESULTS TABLE

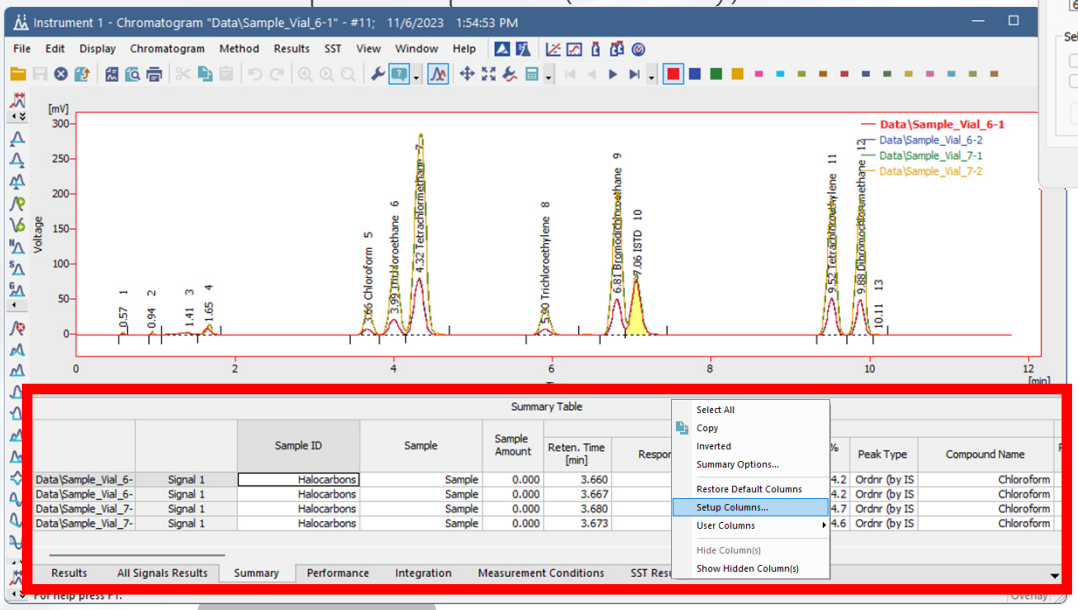
- Results for all signals of selected chromatogram in one table

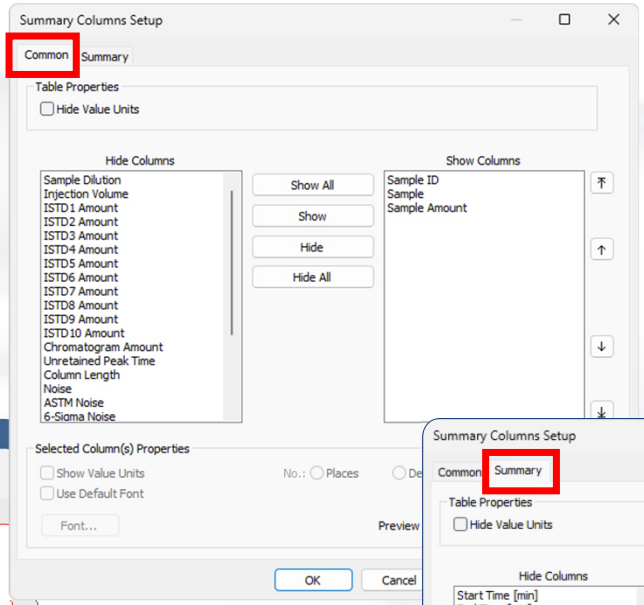


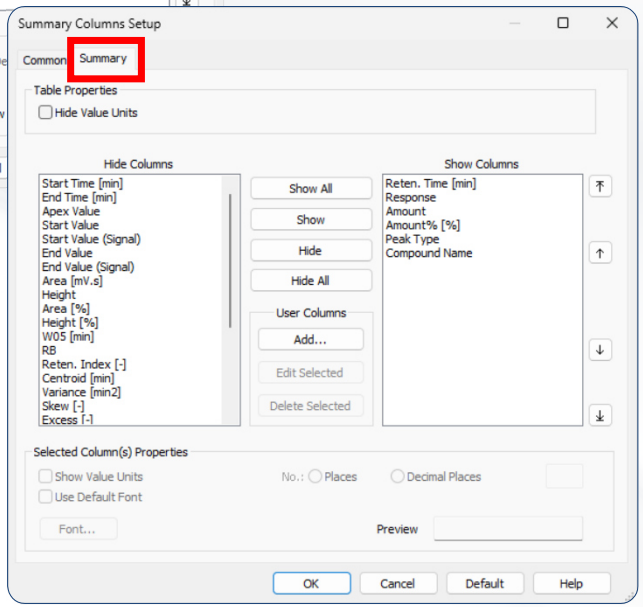
CHROMATOGRAM WINDOW

SUMMARY TABLE

- Summary of all opened chromatograms and signals based on calibration settings
- Setup columns:
  - Common for all compounds
  - Compound-specific (Summary)



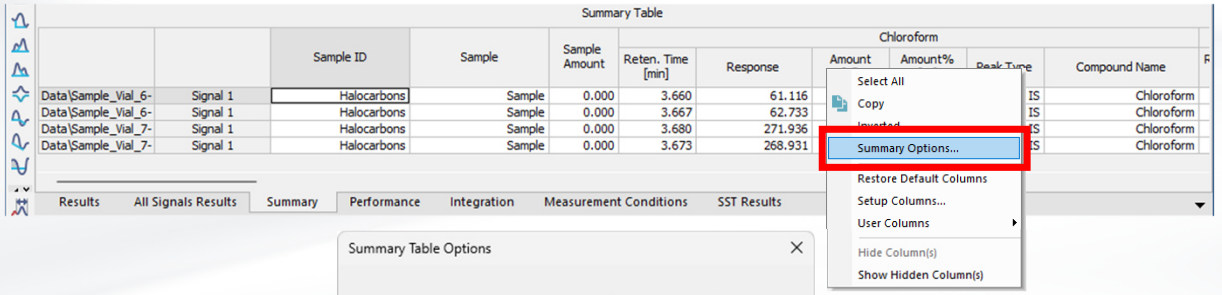


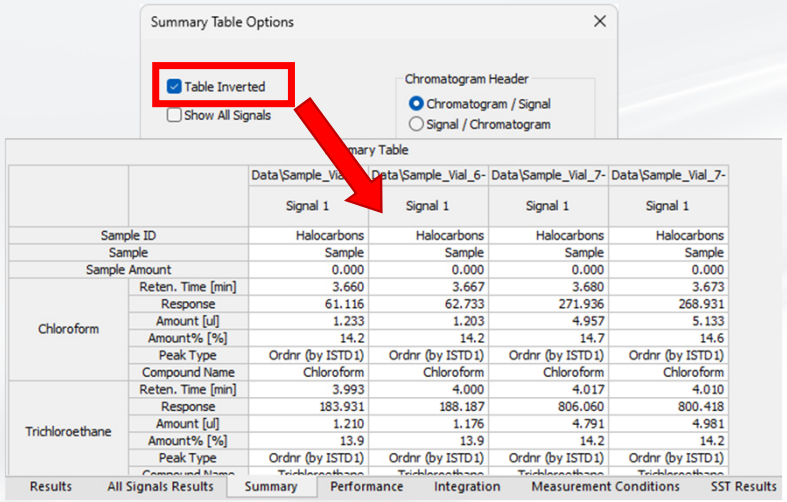


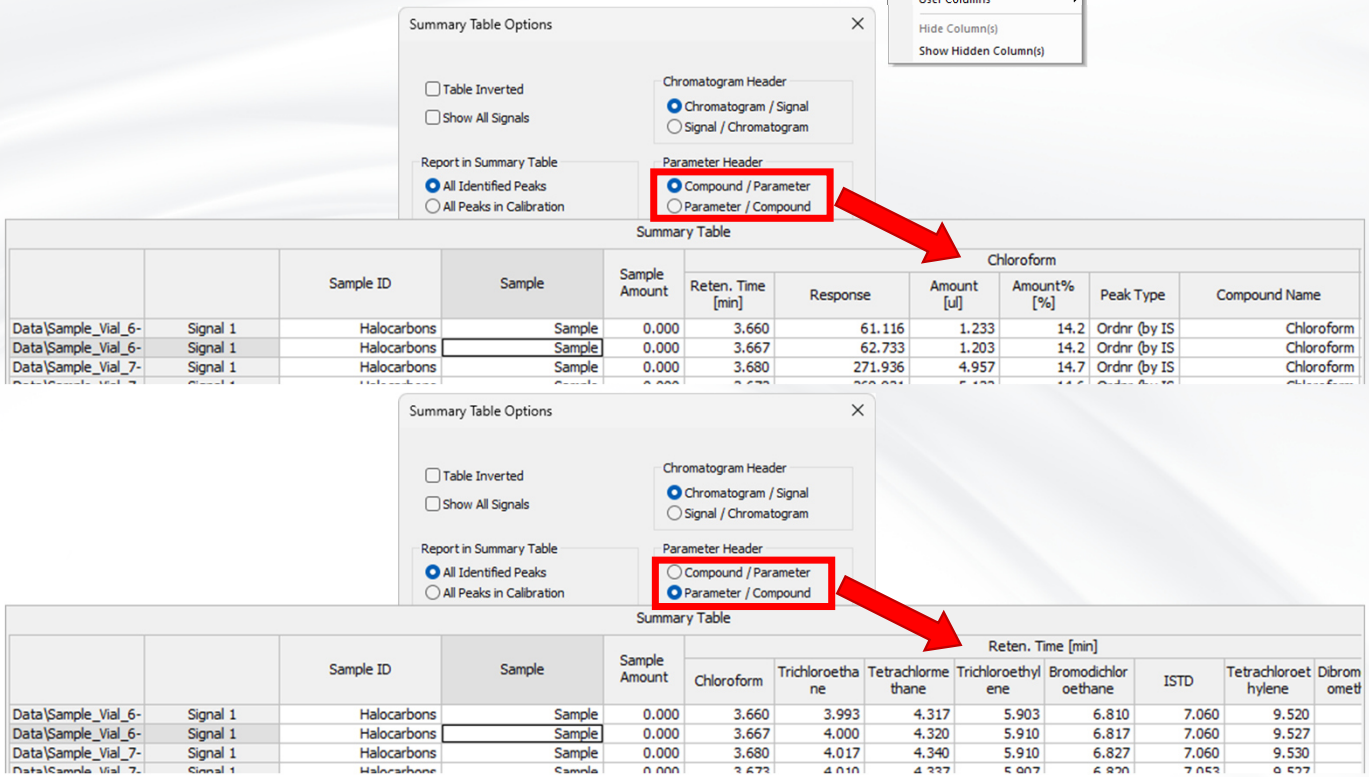
CHROMATOGRAM WINDOW

SUMMARY TABLE OPTIONS

- Accessible through the context menu
- Table inversion, header organization…



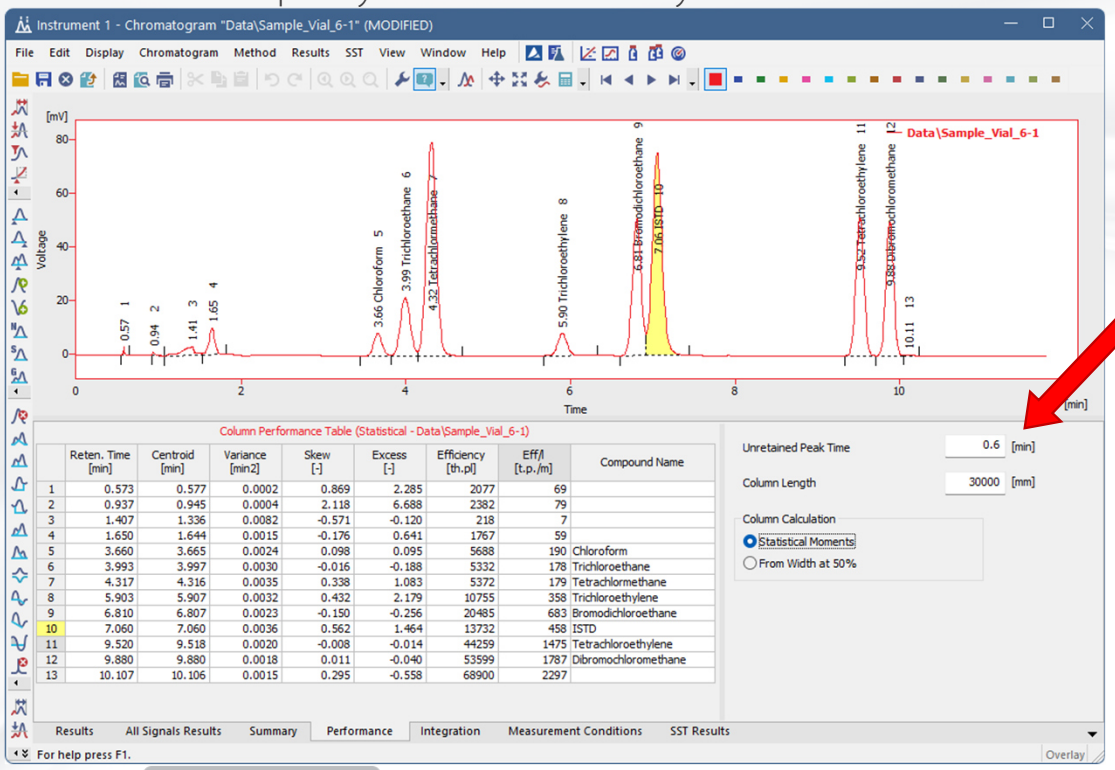


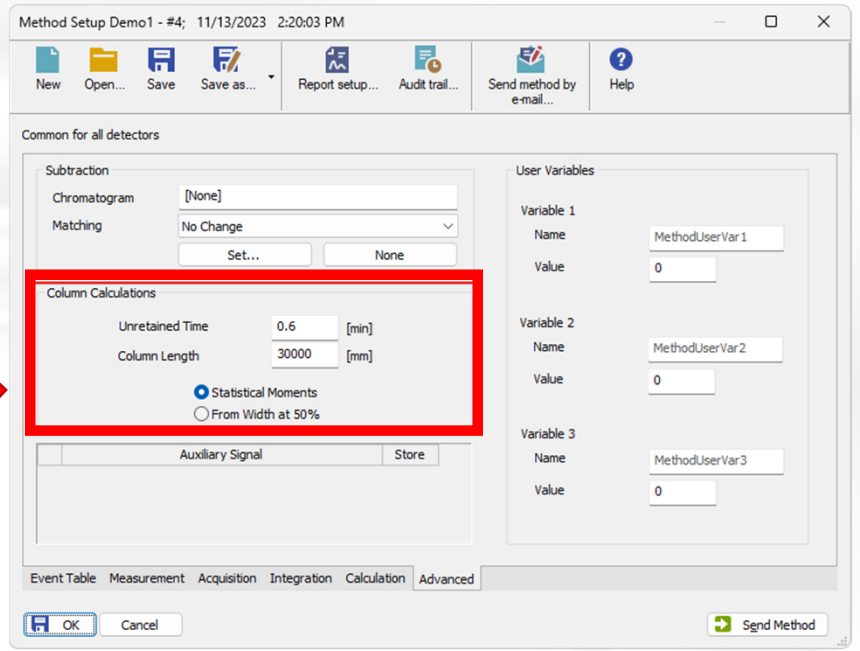


CHROMATOGRAM WINDOW

PERFORMANCE TABLE

- Set calculation type
- Values for capacity ratio and efficiency from the used method

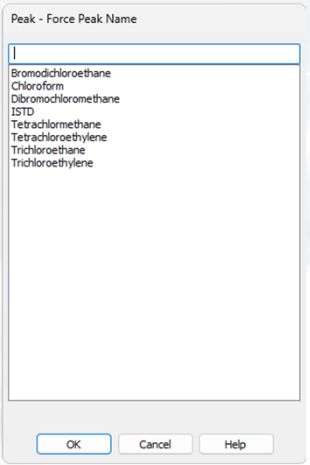


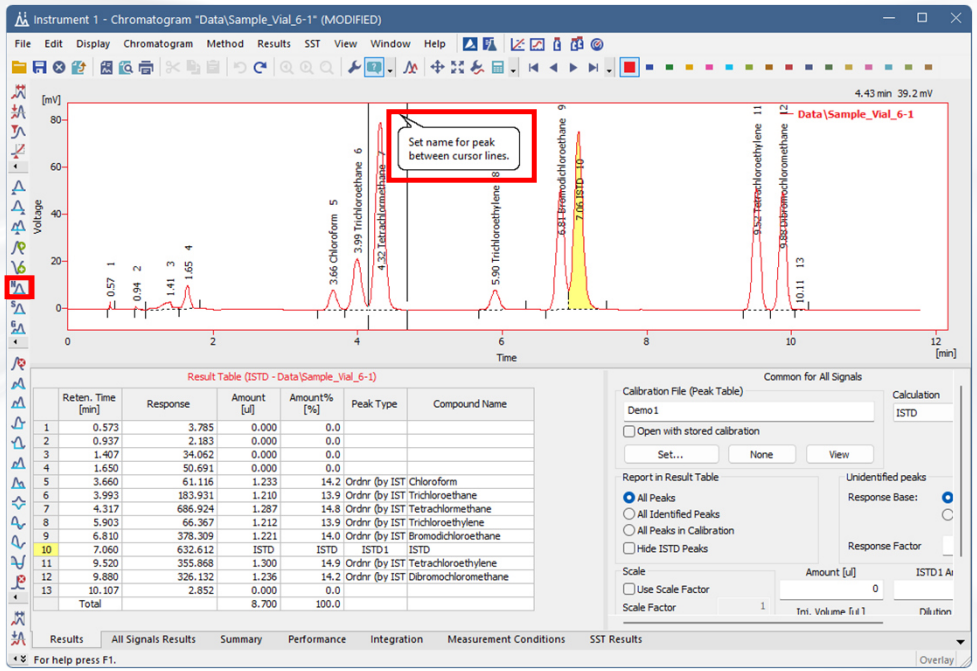


CHROMATOGRAM WINDOW

FORCE PEAK NAME

- Set compound from calibration
- Set custom name

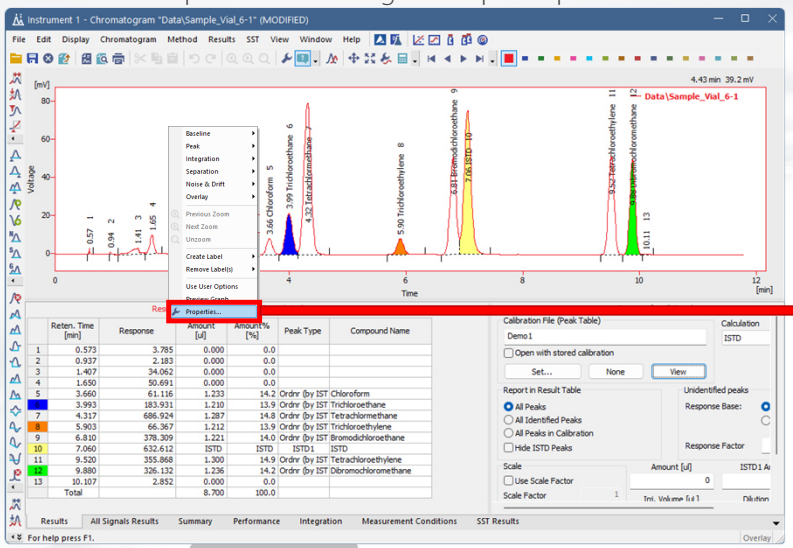


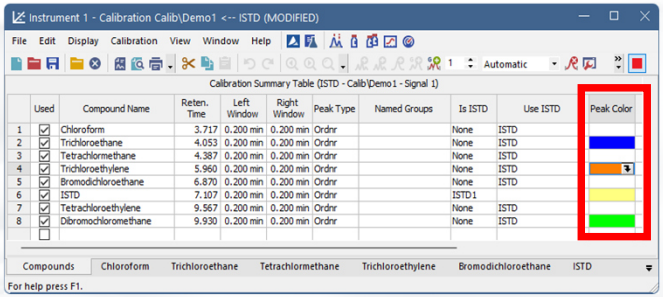


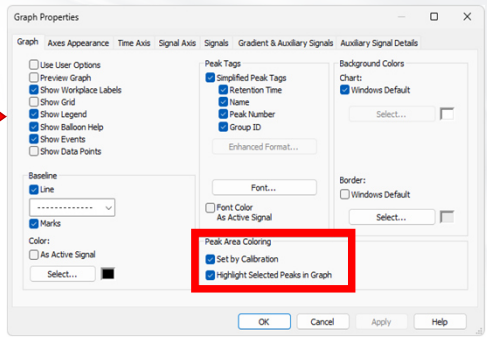
CHROMATOGRAM WINDOW

PEAK COLORS

- Set via Calibration,
- Set peak area coloring via Graph Properties

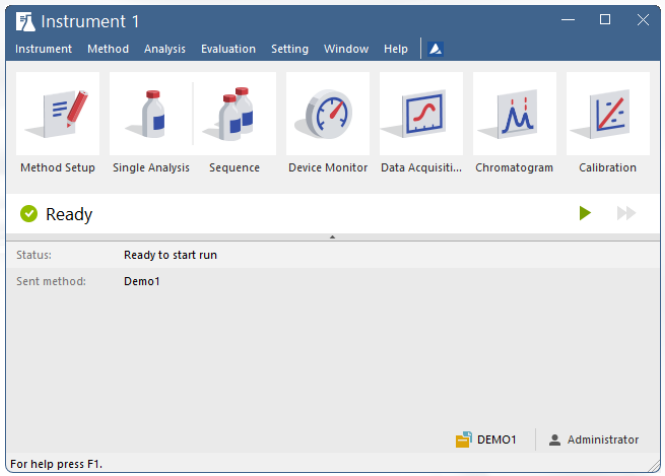






AGENDA

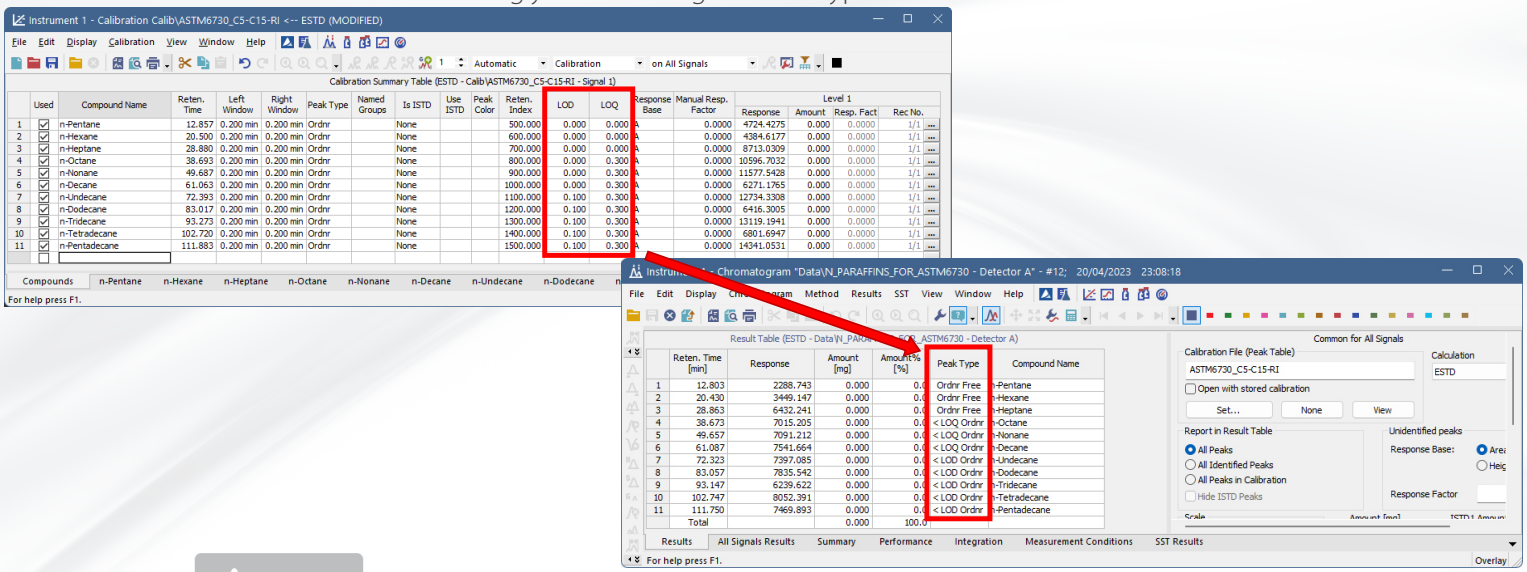
- Chromatogram window
  - Column setup, User columns, Noise & Drift
  - Mathematical operations, Labels
  - Result table, User variables
  - Summary table, Performance table
  - Force peak name, Peak coloring, Graph properties
- Calibration
  - LOD, LOQ
  - Calibration Options, Manual Calibration
  - Details of Calibration Point
  - Bracketing and Standard Addition
- Calculations
  - ISTD, Normalized %
- Groups



CALIBRATION

LOD, LOQ

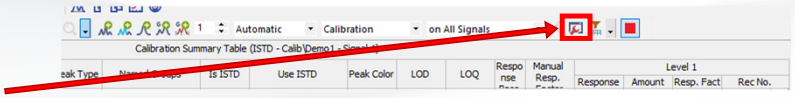
- Limit of Detection (LOD) and Limit of Quantification (LOQ) – amounts lower than LOD/LOQ specified in calibration are marked accordingly in chromatogram Peak Type

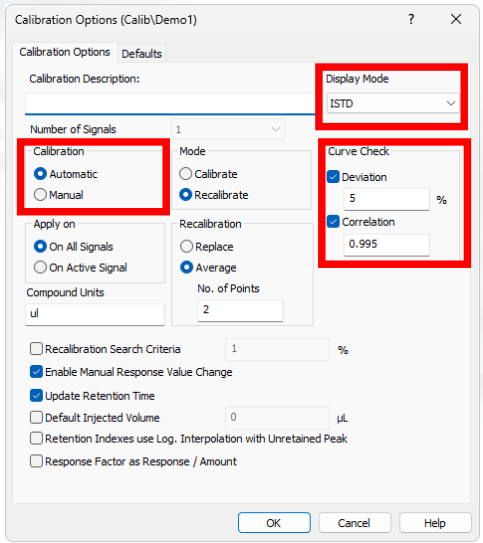


CALIBRATION

CALIBRATION OPTIONS

- Open via *Calibration – Options* or Calibration Options button
- Display Mode – related to calculation types: ESTD, ISTD, NORM, STDADD
- Calibration curve check – threshold used for the **Failure** message in *Result Table – Peak Type*
- Automatic/Manual calibration

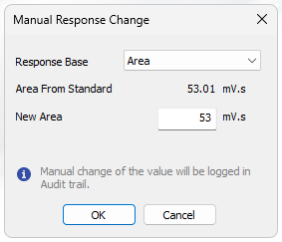


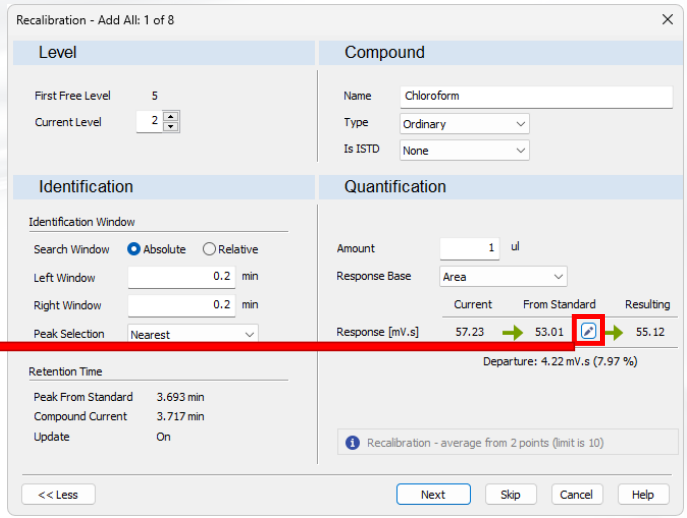


CALIBRATION

MANUAL CALIBRATION

- Accessible when adding points to calibration if Manual calibration is selected in Calibration Options
- You can edit:
  - Calibration level
  - Identification criteria
  - Compound information
  - Response options (Area, Height, or Area %)
- Manual response adjustment

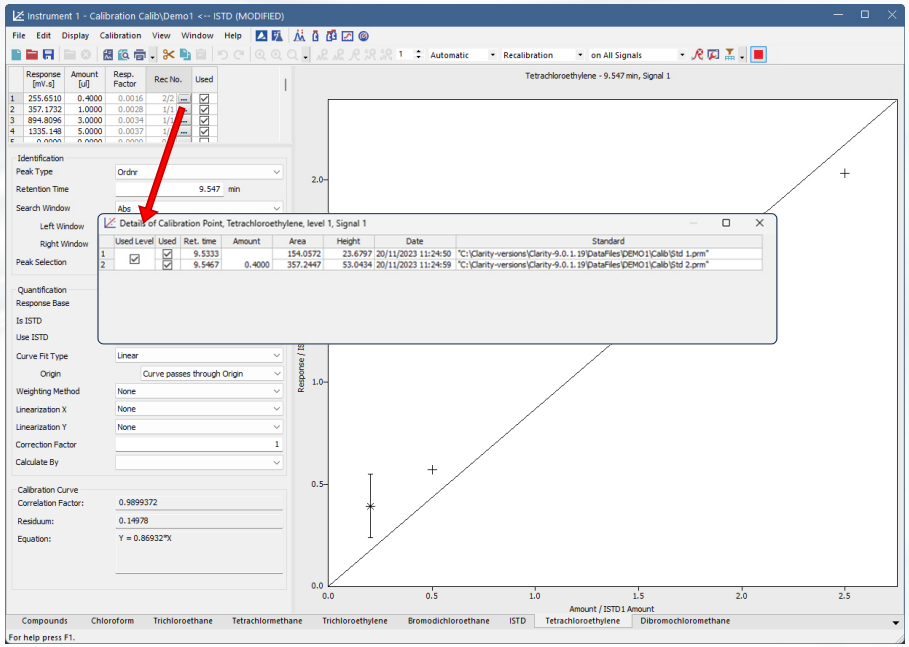




CALIBRATION

DETAILS OF CALIBRATION POINT

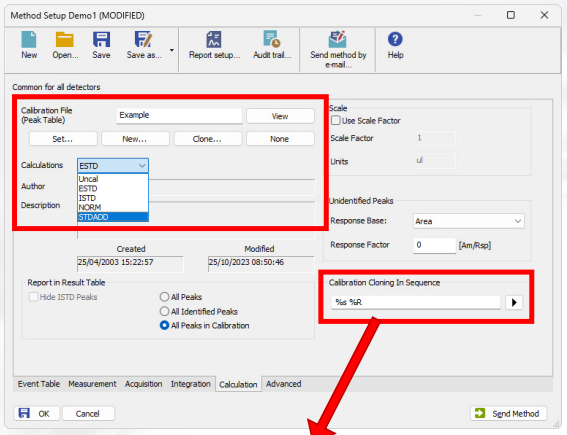
- When recalibrating a level using more points, you can view calibration point details for selected level (accessible also via *Calibration – Show Details*)
- Checkbox state – include/omit from calibration



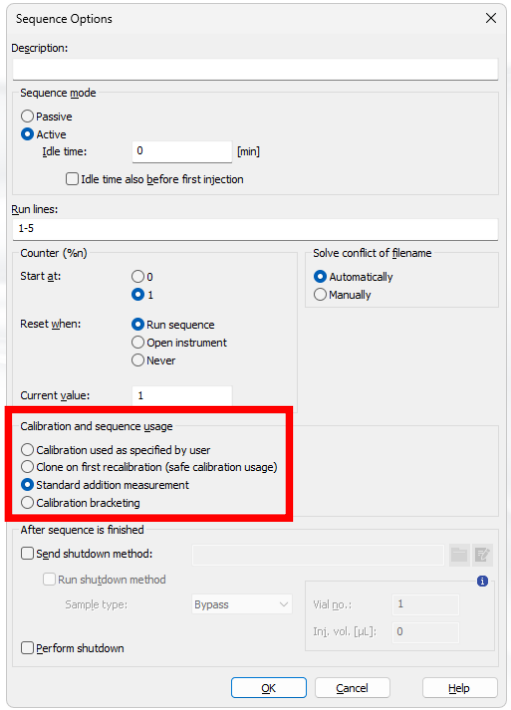
CALIBRATION

BRACKETING AND STANDARD ADDITION

- Calibration in Method is used according to the *Sequence Options – Calibration and sequence usage* option



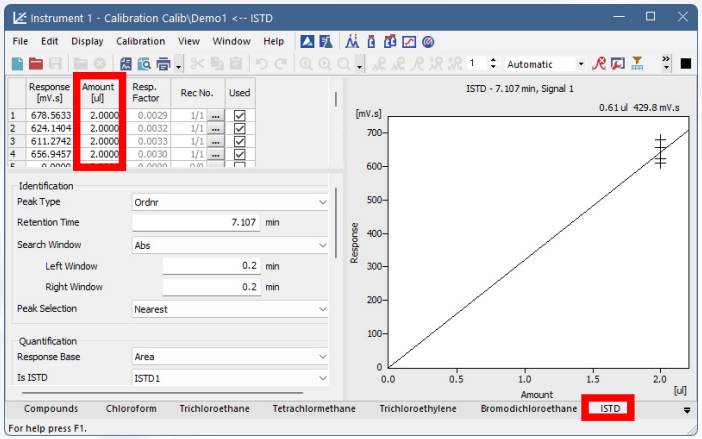
- Name of calibration clone used if the method selected in *Calibration and sequence usage* supports cloning

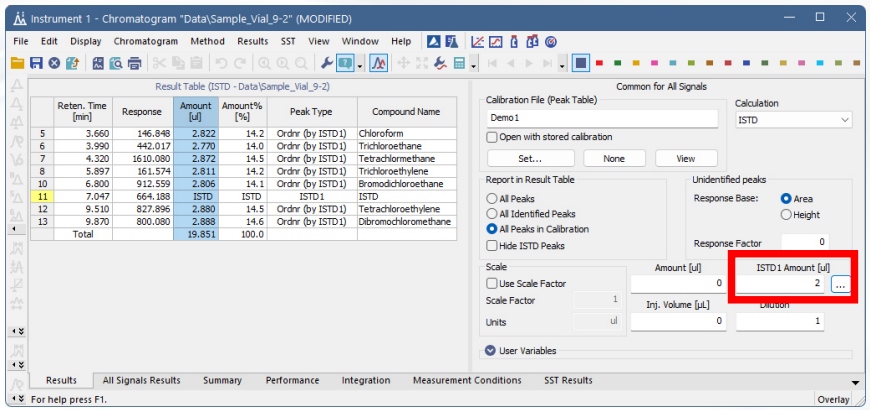


CALCULATIONS

ISTD

- Up to ten ISTD compounds can be present in the calibration/sample
- 2 types of ISTD calculations available:
  - Any amount of ISTD (both calibration and sample chromatogram contain the used ISTD amount)
  - Same amount of ISTD in samples and standards (ISTD amount = 0 in **both** locations)

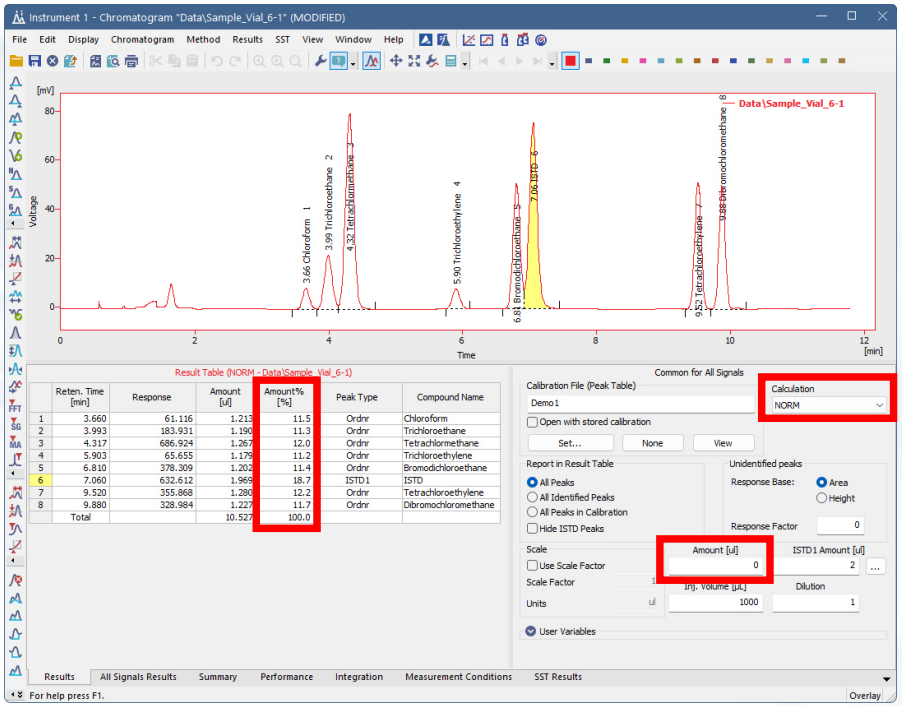




CALCULATIONS

NORMALIZED %

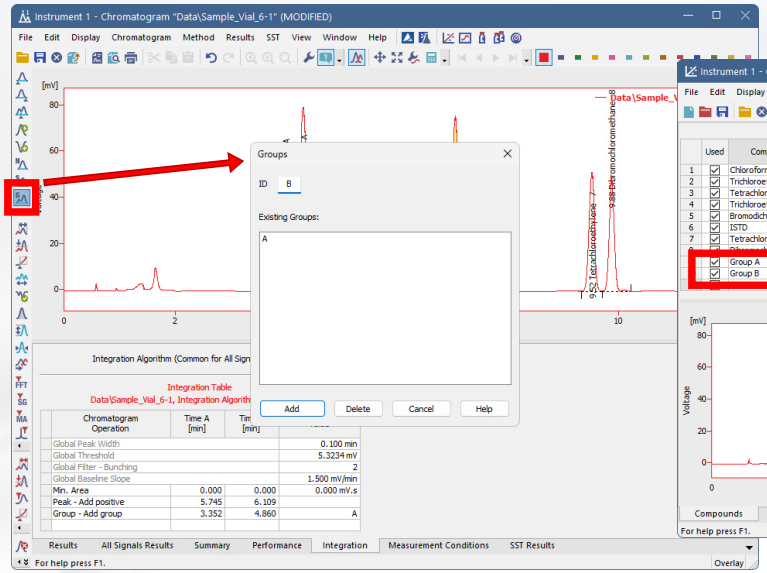
- Amount % column contains the normalized percentage **if all integrated peaks are calibrated**
- If the Sample Amount is 0, compounds in the Amount % column add up to a total of 100%
- Otherwise, the value serves as the total sum of Amount %, and values in the Amount % column are normalized to the Amount set
- NORM is the same as ESTD, except it additionally checks that both all identified peaks are calibrated, **and** all peaks from calibration are identified in the sample chromatogram



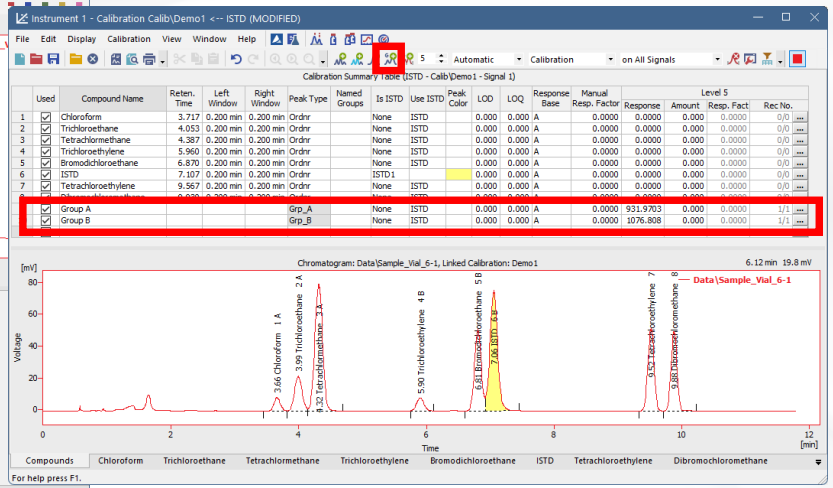
GROUPS

CREATING A GROUP

- Set group ID and add peaks to the group



- Add group in Calibration – set name and amount as for an ordinary peak



Clarity™

ADVANCED CHROMATOGRAPHY SOFTWARE

SHORT BREAK