

23.0331



Clarity™

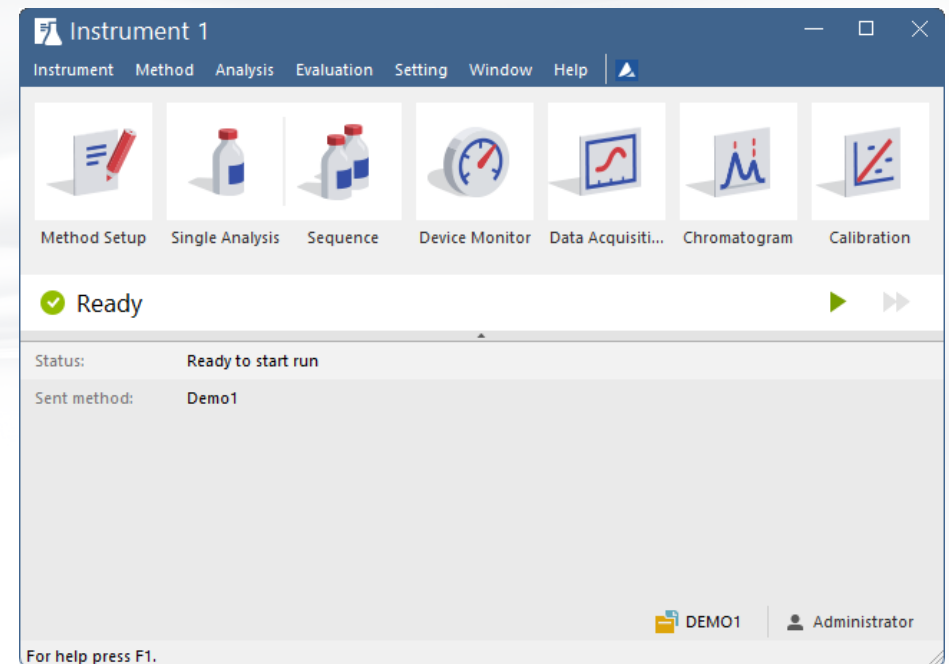
ADVANCED CHROMATOGRAPHY SOFTWARE

CLARITY TRAINING

ADVANCED – PART 2

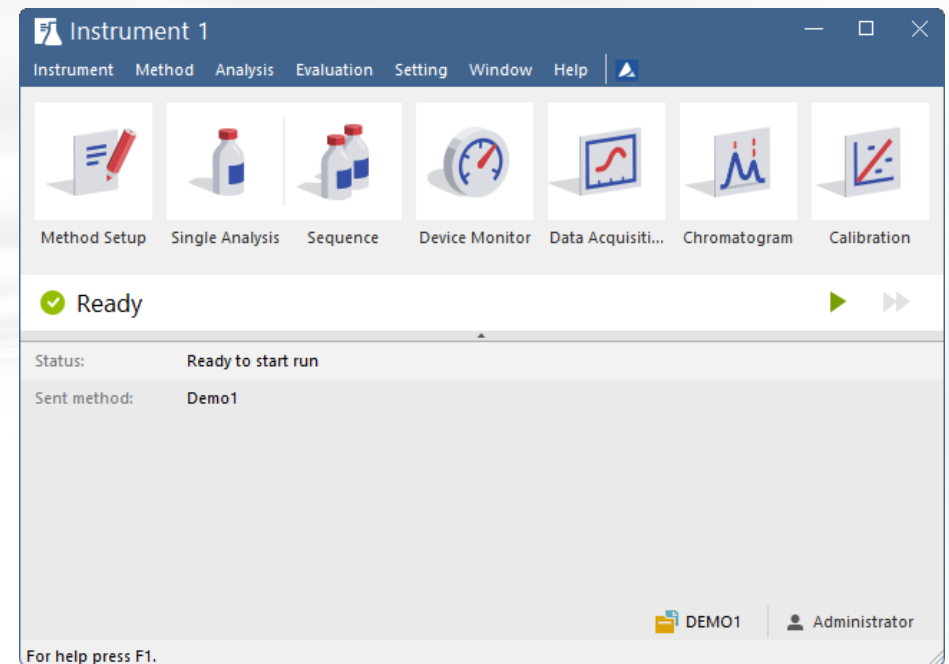
AGENDA

- 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

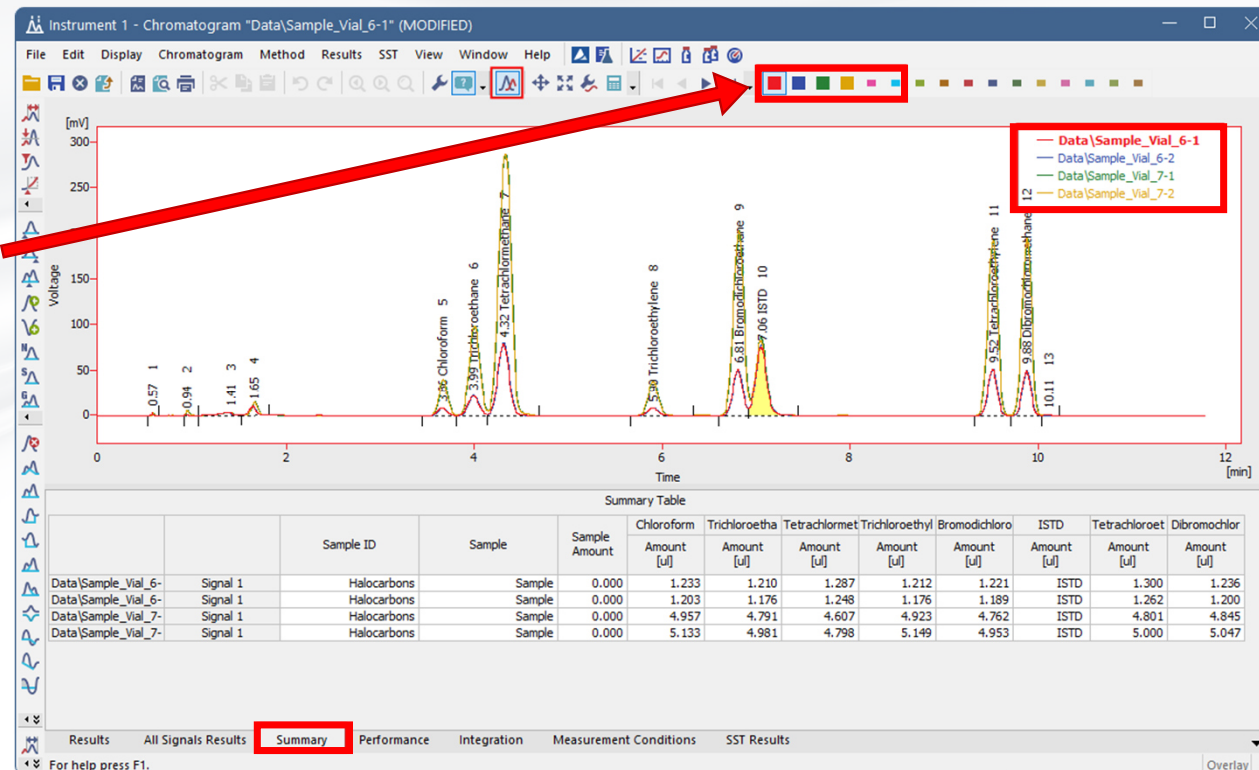
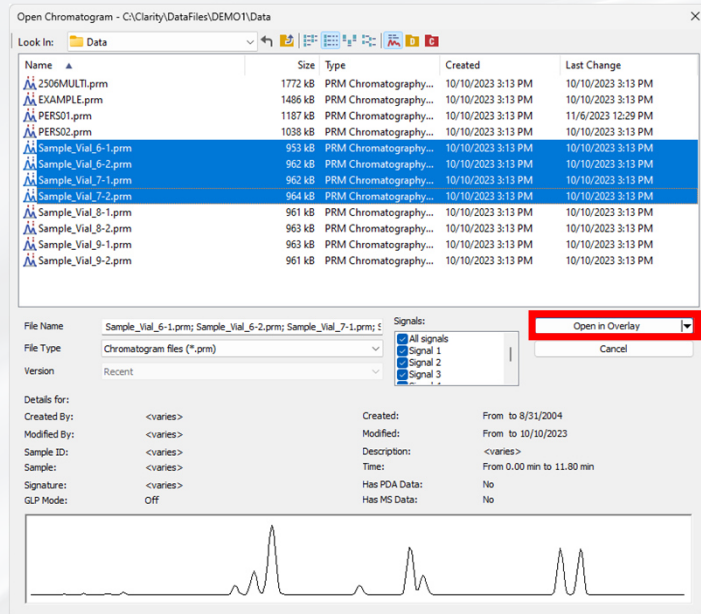
- Chromatogram window
 - Column setup, User columns, Noise & Drift
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 - Result table, User variables
 - Summary table, Performance table
 - Force peak name, Peak coloring, Graph properties
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CHROMATOGRAM WINDOW

OVERLAY

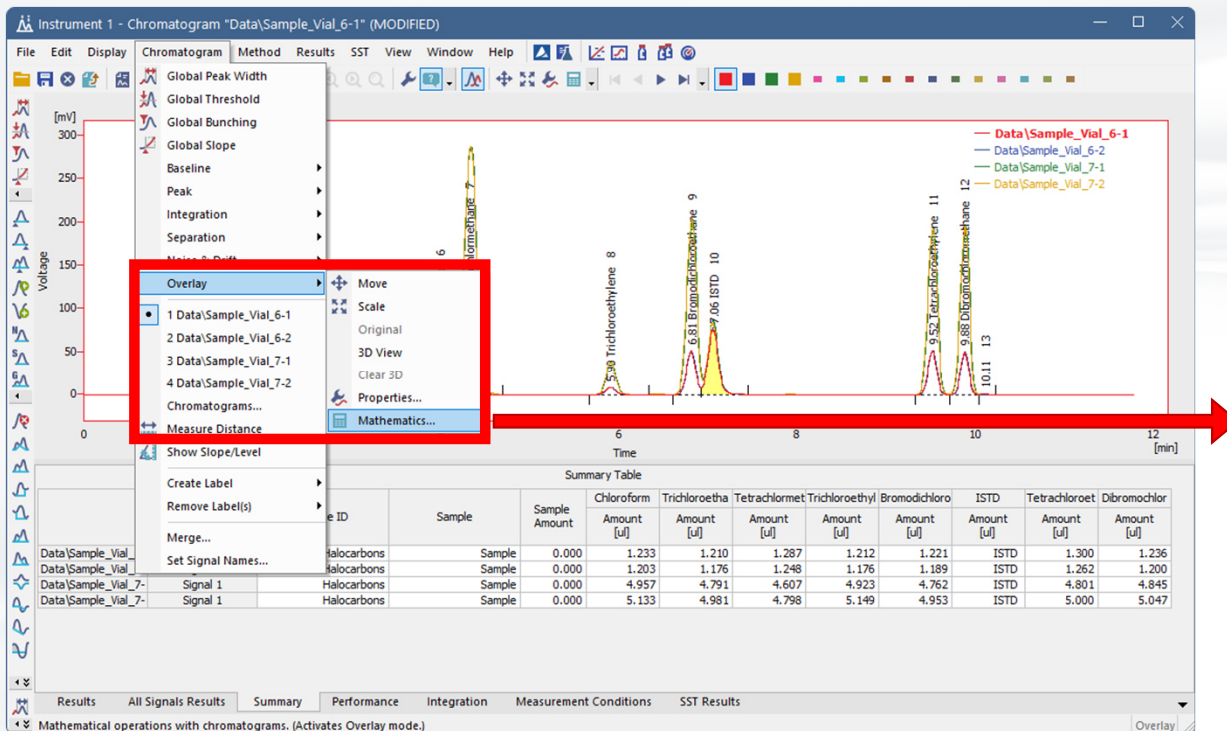
- Comparing multiple chromatograms
 - Max. number is set in User Options
- Summary table shows results of the displayed chromatograms/signals
- Hide/show signals via Ctrl+Click on signal color



CHROMATOGRAM WINDOW

MATHEMATICAL OPERATIONS

- Mathematical operations between signals/chromatograms



The 'Mathematical Operations' dialog box is shown. It allows users to perform mathematical operations on chromatograms. The 'Operand A' is 'Data\Sample_Vial_6-1' and the 'Operand B' is 'Data\Sample_Vial_6-2'. The 'Operation' is 'A + B'. The 'Apply Method' is 'Demo1'. The 'Save As Chromatogram' checkbox is checked. The 'OK', 'Cancel', and 'Help' buttons are at the bottom.

CHROMATOGRAM WINDOW

LABELS

- Add text labels or lines

Text Label

Text
My Label

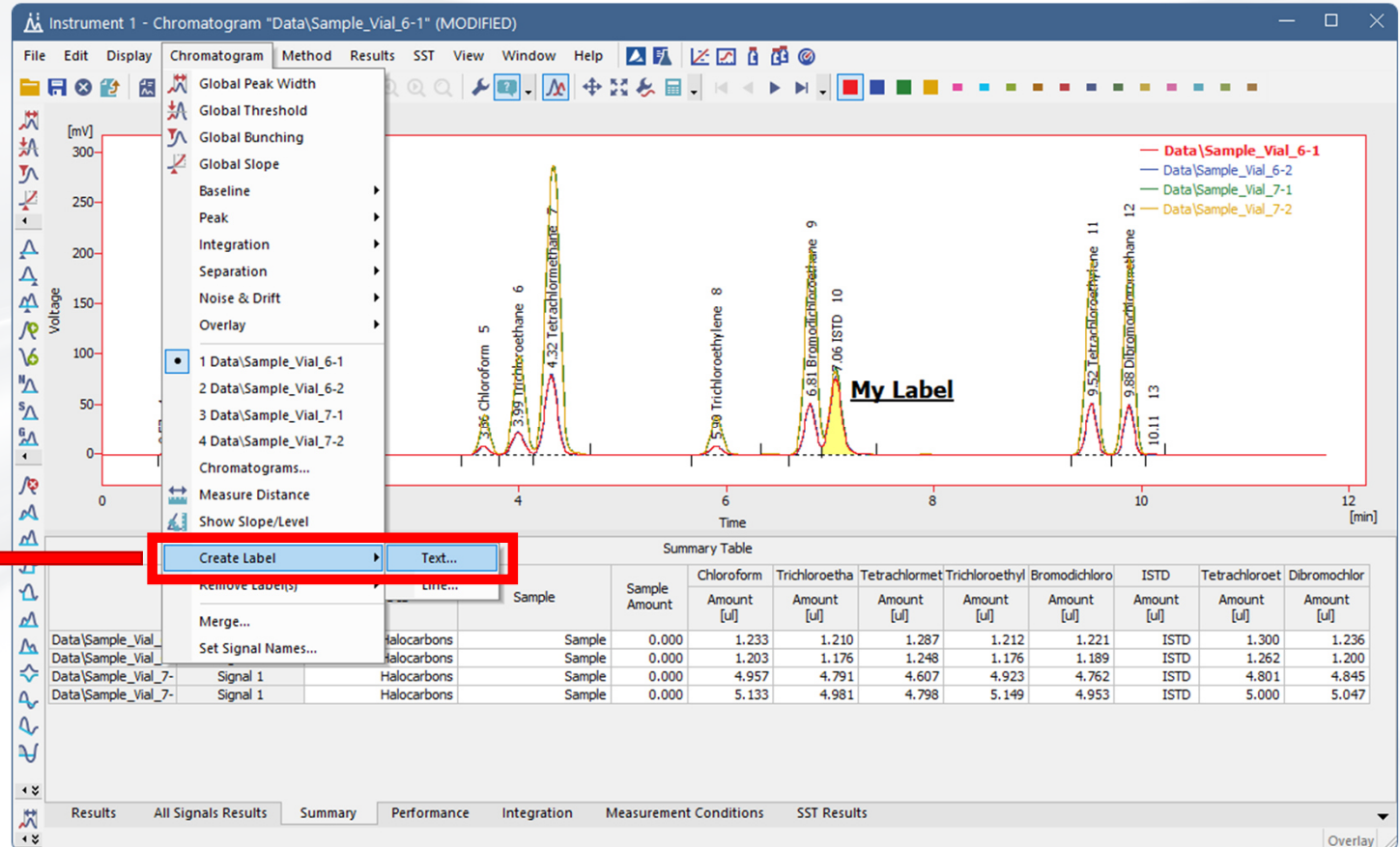
Orientation
0 degrees

Font...

Assign to
☒ Workplace
☐ Active Signal

Anchor (Text Alignment)
☒ Text Alignment

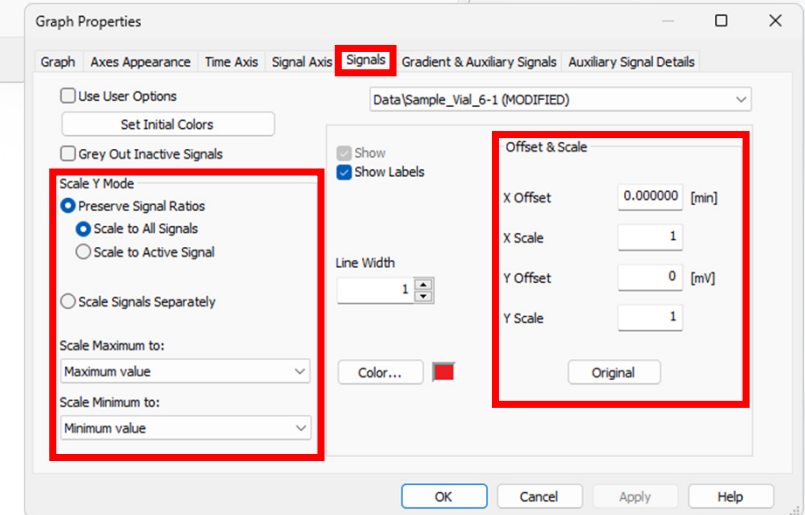
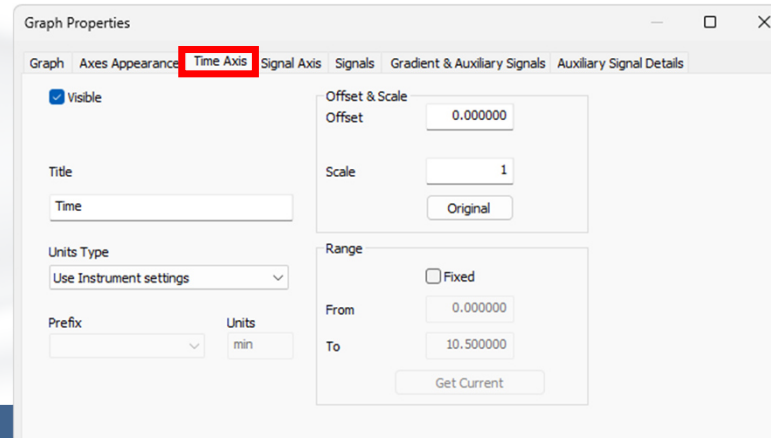
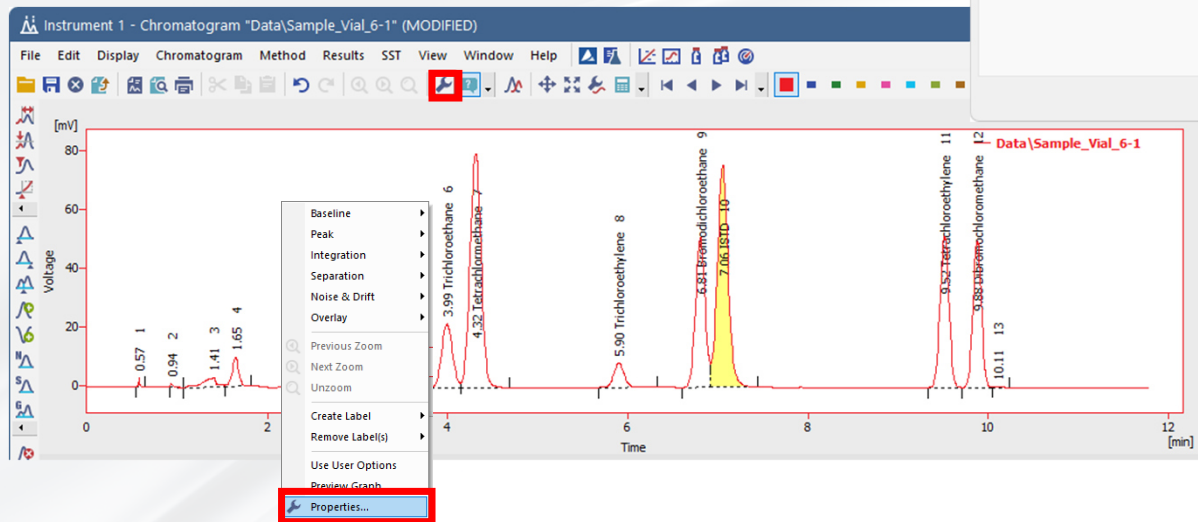
OK
Cancel
Help
Delete



CHROMATOGRAM WINDOW

GRAPH PROPERTIES

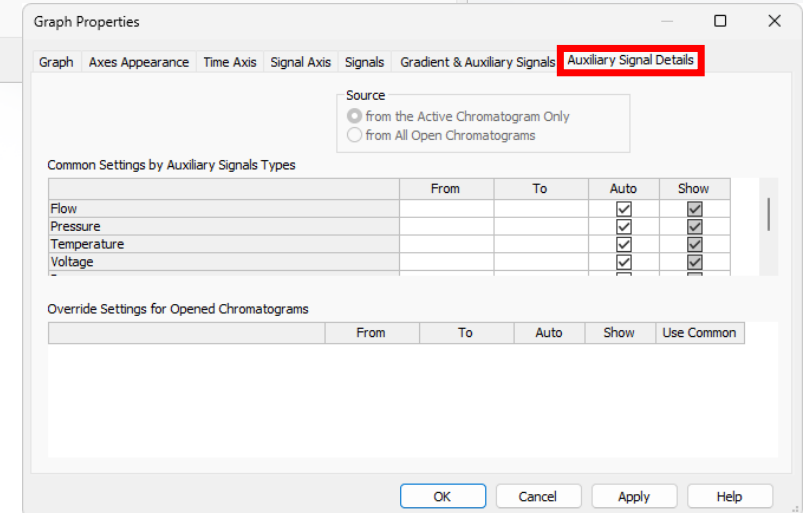
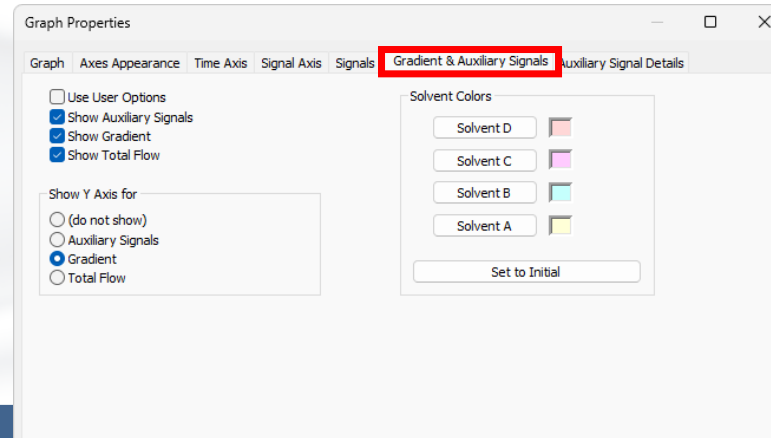
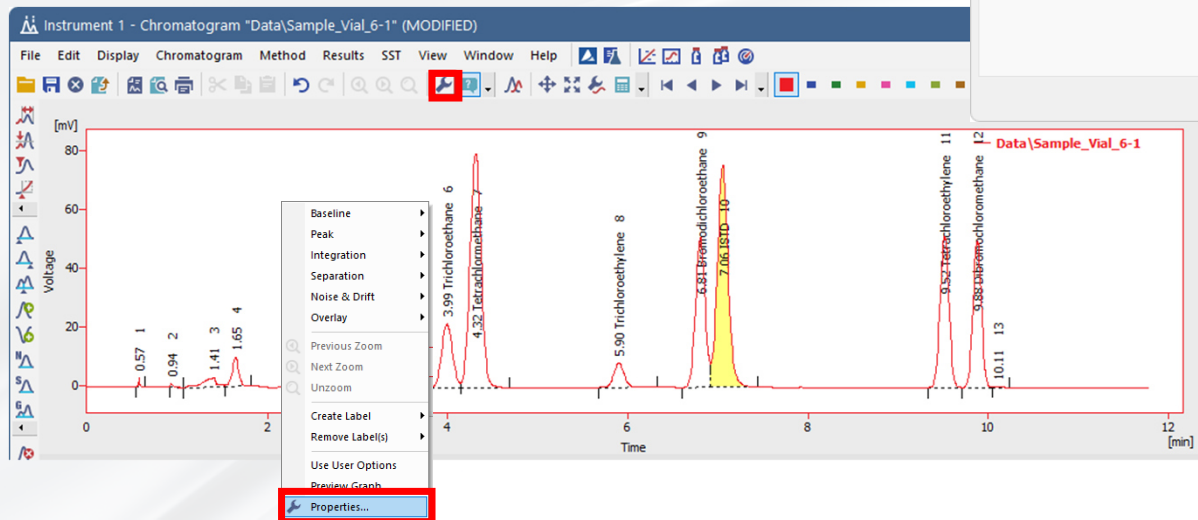
- Axis settings
- Signal scaling –general settings, settings for individual signals



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

Result Table (ISTD - Data\Sample_Vial_6-2)

	Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
1	0.580	3.963	0.000	0.0		
2	0.940	2.035	0.000	0.0		
3	1.400	35.640	0.000	0.0		
4	1.650	51.550	0.000	0.0		
5	3.667	62.733				oform
6	4.000	188.187				loroethane
7	4.320	701.151				achlormethane
8	5.910	67.722				loroethylene
9	6.817	387.435				odichloroethane
10	7.060	665.757				
11	9.527	363.746				achloroethylene
12	9.887	333.096				omochloromethane
13	10.107	2.966				
Total						

Context Menu:

- Select All
- Copy
- Restore Default Columns
- Setup Columns...
- User Columns
- Hide Column(s)
- Show Hidden Column(s)

Results | All Signals Results | Summary | Performance | Integration | Measurement Conditions | SST Result

Setup columns

Setup Columns

Table Properties

☐ Hide Value Units

Hide Columns

Start Time [min]
End Time [min]
Apex Value [mV]
Start Value [mV]
Start Value (Signal) [mV]
End Value [mV]
End Value (Signal) [mV]
Area [mV.s]
Height [mV]
Area [%]
Height [%]
W05 [min]
RB
Reten. Index [-]
Centroid [min]
Variance [min²]
Skew [-]
Excess [-]

Show All
Show
Hide
Hide All

User Columns

Add...
Edit Selected
Delete Selected

Show Columns

Reten. Time [min]
Response
Amount [ul]
Amount% [%]
Peak Type
Compound Name

Selected Column(s) Properties

☐ Show Value Units
☒ Use Default Font

No.: ☐ Places ☒ Decimal Places 3

Font... Preview 123.457

OK Cancel Default Help

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

Result Table (ESTD - Data\2506MULTI - UV)

	Reten. Time [min]	Response	Amount [g/l]	Amount% [%]	Peak Type	Compound Name
1	4.565	3.408	0.025	0.3	Ordnr	oxalic
2	5.200				Ordnr	citric
3	5.415				Ordnr	tartaric
4	6.300				Ordnr	malic
8	8.160				Ordnr	succinic
9	8.550				Ordnr	lactic
11	10.345				Ordnr	acetic
C11	12.710					methanol
Total						

Results All Signals Results Summary Performance

Add User Column

Add User Column

Title: RRT Units:

☒ Calculate Total

Expression:

OK Cancel Help

Ops:

Funcs:

Columns:

Variables:

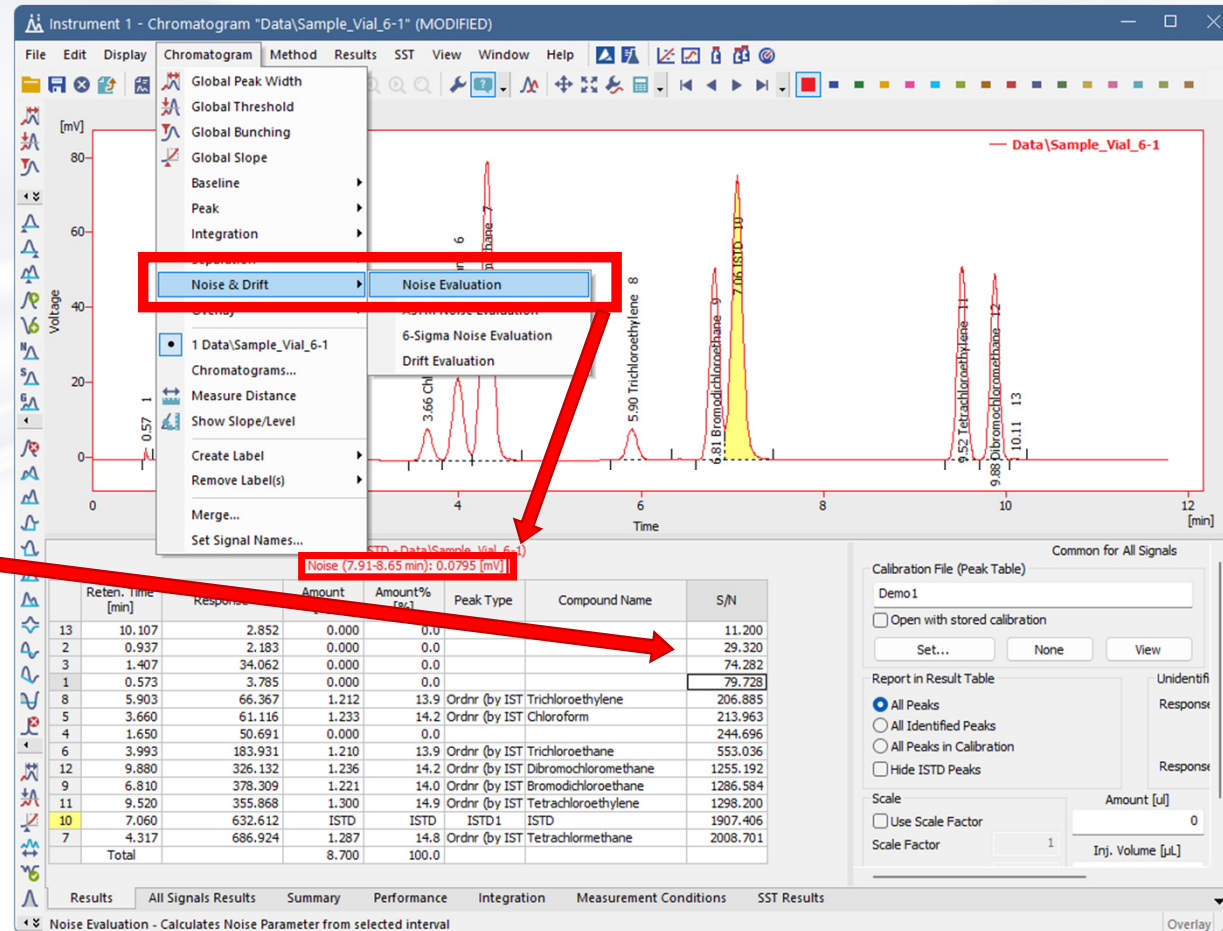
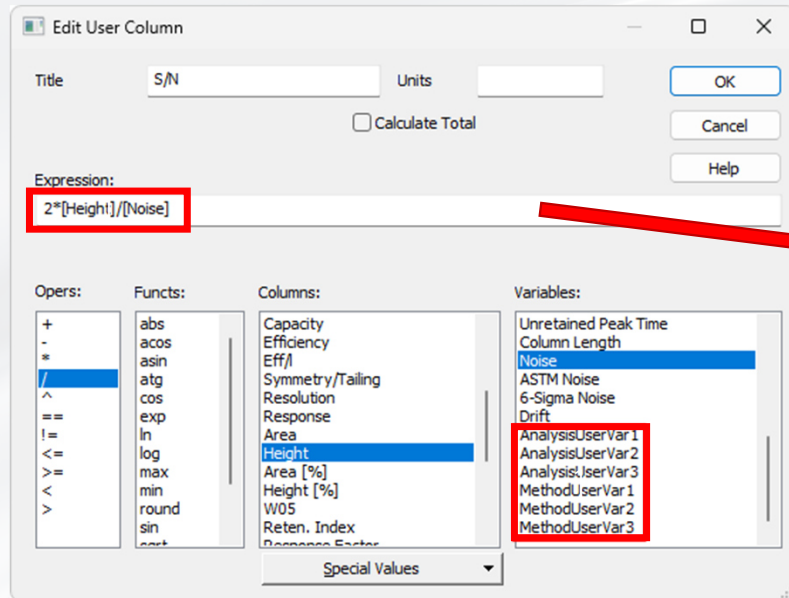
- Special Values
- Sum
 - Average
 - Std. Deviation
 - Minimum
 - Maximum
 - First
 - Last
 - Previous
 - Next
 - Compound

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
Compound	11.778

CHROMATOGRAM WINDOW

USER COLUMNS – NOISE & DRIFT

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



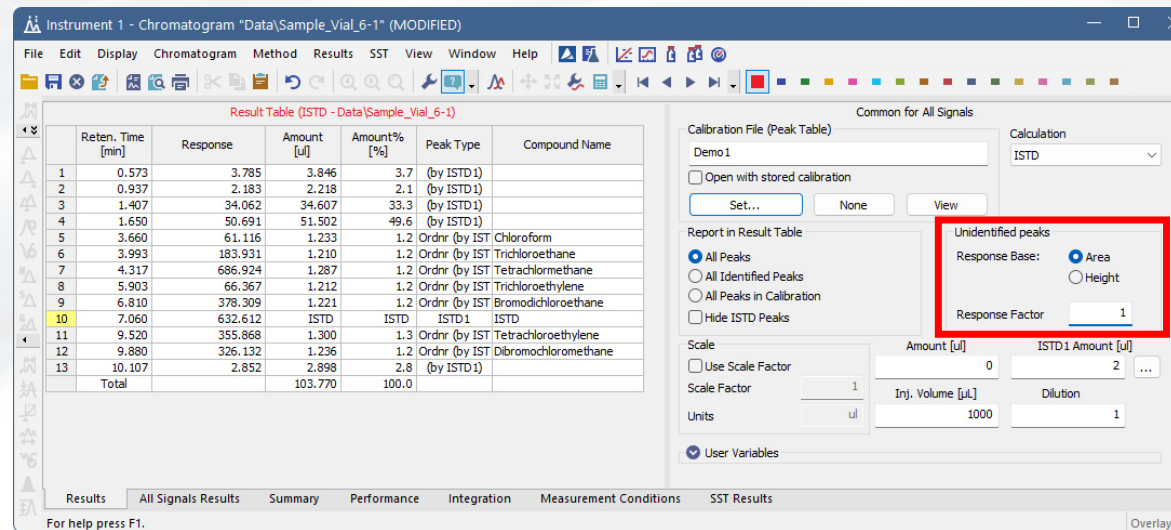
CHROMATOGRAM WINDOW

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:

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

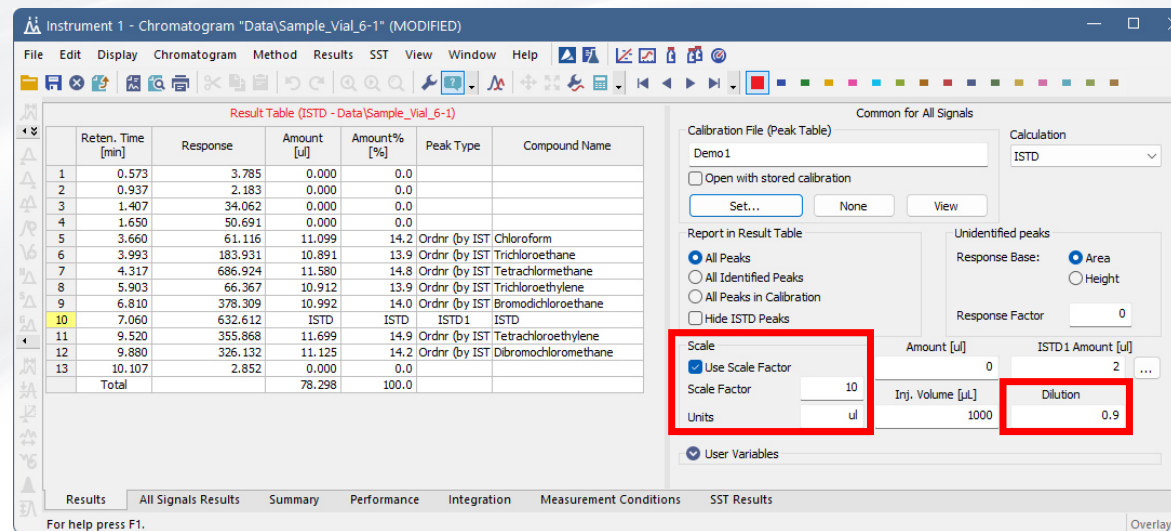
- Provides a “single-point quantification” of unidentified compounds (e.g., for universal response detectors like ELSD, FID, RI, etc.)



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

Instrument 1 - Chromatogram "Data\Sample_Vial_6-1" - #12; 21/11/2023 11:20:26

File Edit Display Chromatogram Method Results SST View Window Help

Result Table (ISTD - Data\Sample_Vial_6-1)

	Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
4	3.660	61.116	1.233	14.2	Ordnr (by ISTD 1)	Chloroform
5	3.993	183.931	1.210	13.9	Ordnr (by ISTD 1)	Trichloroethane
6	4.317	686.924	1.287	14.8	Ordnr (by ISTD 1)	Tetrachloromethane
7	5.903	65.887	1.204	13.8	Ordnr (by ISTD 1)	Trichloroethylene
8	6.810	378.309	1.221	14.0	Ordnr (by ISTD 1)	Bromodichloroethane
9	7.060	632.612	ISTD	ISTD	ISTD 1	ISTD
10	9.520	355.868	1.300	14.9	Ordnr (by ISTD 1)	Tetrachloroethylene
11	9.880	328.984	1.247	14.3	Ordnr (by ISTD 1)	Dibromochloromethane
Total			8.702	100.0		

Common for All Signals

Calibration File (Peak Table) Demo1 Calculation ISTD

☐ Open with stored calibration

Set... None View

Report in Result Table

☐ All Peaks
☒ All Identified Peaks
☐ All Peaks in Calibration
☐ Hide ISTD Peaks

Unidentified peaks

Response Base: ☒ Area ☐ Height

Response Factor 0

Scale

☐ Use Scale Factor

Scale Factor 1

Units ul

Inj. Volume [uL] 1000 Dilution 1

User Variables

Analysis Variables

Name	Value
1 My Variable 1	10
2 My Variable 2	20
3 My Variable 3	-20

Method Variables

Name	Value
1 MethodUserVar1	0
2 MethodUserVar2	0
3 MethodUserVar3	0

Single Analysis

Variable	Name	Value
Variable 1	My Variable 1	10
Variable 2	My Variable 2	20
Variable 3	My Variable 3	-20

Analysis Post Run Settings User Variables

Control

Send method Inject & Run Stop Abort Snapshot

☒ Use Autosampler Vial 1

Chromatogram File Name (Calib\Instrument 1 - 21_11_2023 11_14_44)

%e - %R

☐ Enable File Overwrite Counter 1 Data Recovery...

OK Cancel Help

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

The screenshot displays two windows from the DataApex software. The 'Instrument 1 - Chromatogram' window shows a 'Result Table (ISTD - Data\Sample_Vial_6-1)' with columns for Reten. Time, Response, Amount, Amount%, Peak Type, and Compound Name. The 'Instrument 1 - Sequence Demo1 (MODIFIED)' window shows a table with columns for Status, Run, SV, EV, I/V, Sample ID, Sample, Sample Amount, ISTD1 Amount, Sample Dilut., Inj. Vol., and three custom variables: My Variable 1, My Variable 2, and My Variable 3. A red box highlights these three columns. A red arrow points from this box to the 'User Variables' section in the 'Chromatogram' window, which also has a red box around it. The 'User Variables' section shows 'Analysis Variables' and 'Method Variables' with their respective names and values.

Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
4	3.660	61.116	1.233	14.2	Ordnr (by ISTD1) Chloroform
5	3.993	183.931	1.210	13.9	Ordnr (by ISTD1) Trichloroethane
6	4.317	686.924	1.287	14.8	Ordnr (by ISTD1) Tetrachloromethane
7	5.903	65.887	1.204	13.8	Ordnr (by ISTD1) Trichloroethylene
8	6.810	378.309	1.221	14.0	Ordnr (by ISTD1) Bromodichloroethane
9	7.060	632.612	ISTD	ISTD	ISTD
10	9.520	355.868	1.300	14.9	Ordnr (by ISTD1) Tetrachloroethylene
11	9.880	328.984	1.247	14.3	Ordnr (by ISTD1) Dibromochloromethane
Total		8.702	100.0		

Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj. Vol. [ul]	My Variable 1	My Variable 2	My Variable 3	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1	✓	1:A1	1:A1	1	Halocarbons	Std_1	0.400	2.000	1.000	5.00	10.000	20.000	-20.000	%Q	Stan	1	Demo1	Calibration			
2	✓	1:B1	1:B1	1	Halocarbons	Std_2	1.000	2.000	1.000	5.00	10.000	20.000	-20.000	%Q	Stan	2	Demo1	Calibration			
3	✓	1:C1	1:C1	1	Halocarbons	Std_3	3.000	2.000	1.000	5.00	10.000	20.000	-20.000	%Q	Stan	3	Demo1	Calibration			
4	✓	1:D1	1:D1	1	Halocarbons	Std_4	5.000	2.000	1.000	5.00	10.000	20.000	-20.000	%Q	Stan	4	Demo1	Calibration		✓	
5	✓	1:E1	1:B2	2	Halocarbons	Sample	5.000	2.000	1.000	5.00	10.000	20.000	-20.000	%Q	Unkn		Demo1	Analysis	✓		

Analysis Variables		Method Variables	
Name	Value	Name	Value
1 My Variable 1	10	1 MethodUserVar 1	0
2 My Variable 2	20	2 MethodUserVar 2	0
3 My Variable 3	-20	3 MethodUserVar 3	0

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

The screenshot shows the 'Instrument 1 - Chromatogram' window. The 'Result Table (ISTD - Data\Sample_Vial_6-1)' is displayed with the following data:

	Reten. Time [min]	Response	Amount [uL]	Amount% [%]	Peak Type	Compound Name
4	3.660	61.116	1.233	14.2	Ordnr (by ISTD 1)	Chloroform
5	3.993	183.931	1.210	13.9	Ordnr (by ISTD 1)	Trichloroethane
6	4.317	686.924	1.287	14.8	Ordnr (by ISTD 1)	Tetrachloromethane
7	5.903	65.887	1.204	13.8	Ordnr (by ISTD 1)	Trichloroethylene
8	6.810	378.309	1.221	14.0	Ordnr (by ISTD 1)	Bromodichloroethane
9	7.060	632.612	ISTD	ISTD	ISTD 1	ISTD
10	9.520	355.868	1.300	14.9	Ordnr (by ISTD 1)	Tetrachloroethylene
11	9.880	328.984	1.247	14.3	Ordnr (by ISTD 1)	Dibromochloromethane
Total			8.702	100.0		

The 'Method Variables' table is also shown, which is highlighted with a red box:

Name	Value
1 My Method Variable 1	40
2 My Method Variable 2	50
3 My Method Variable 3	-60

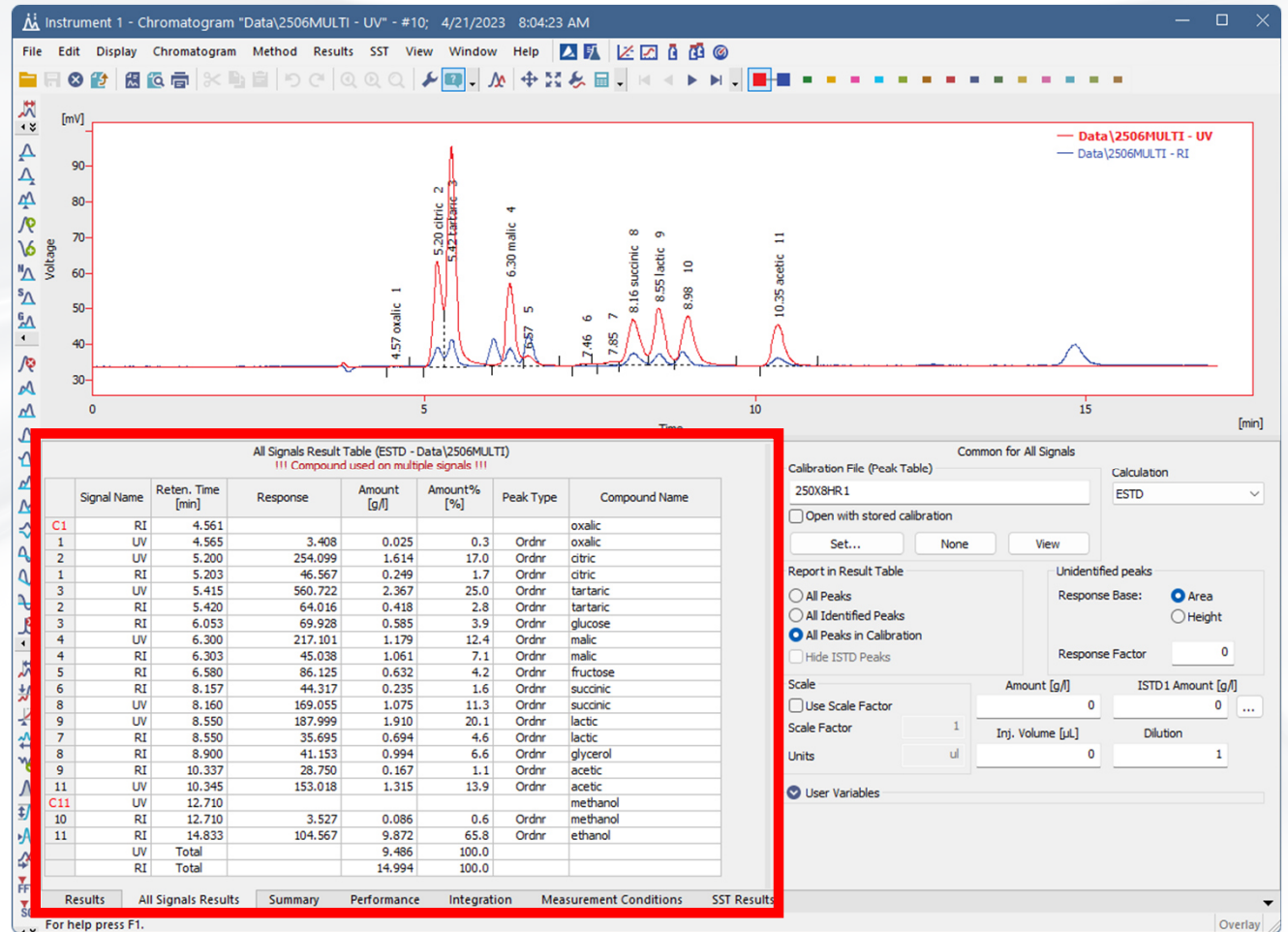
The screenshot shows the 'Method Setup Demo1 (MODIFIED)' window. The 'User Variables' section is highlighted with a red box:

Variable	Name	Value
Variable 1	My Method Variable 1	40
Variable 2	My Method Variable 2	50
Variable 3	My Method Variable 3	-60

CHROMATOGRAM WINDOW

ALL SIGNALS RESULTS TABLE

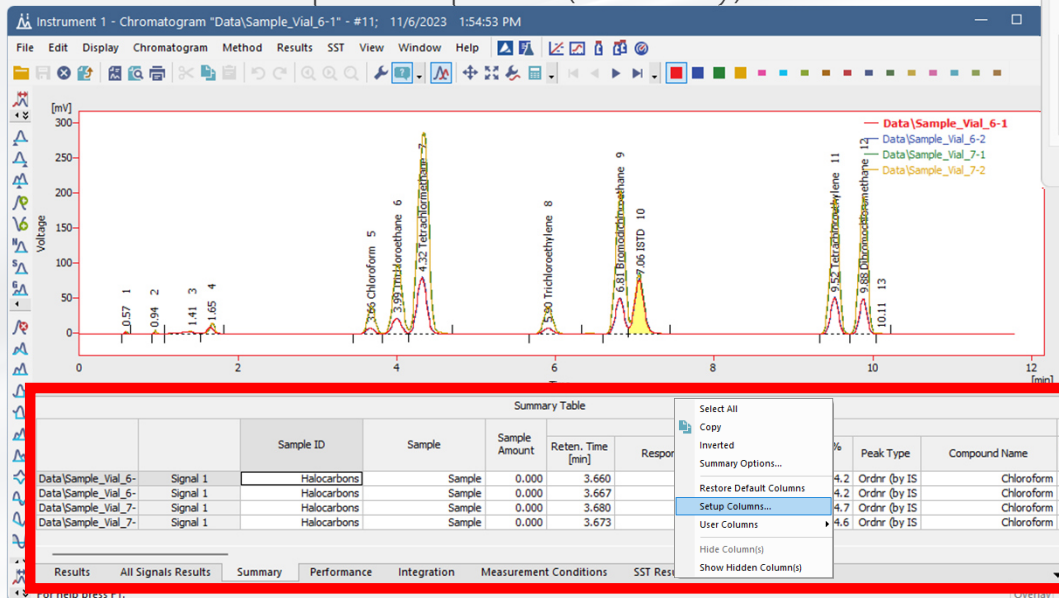
- Results for all signals of selected chromatogram in one table



CHROMATOGRAM WINDOW

SUMMARY TABLE

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



Summary Columns Setup

Common Summary

Table Properties

☐ Hide Value Units

Hide Columns

Sample Dilution
Injection Volume
ISTD 1 Amount
ISTD 2 Amount
ISTD 3 Amount
ISTD 4 Amount
ISTD 5 Amount
ISTD 6 Amount
ISTD 7 Amount
ISTD 8 Amount
ISTD 9 Amount
ISTD 10 Amount
Chromatogram Amount
Unretained Peak Time
Column Length
Noise
ASTM Noise
6-Sigma Noise

Show All
Show
Hide
Hide All

Show Columns

Sample ID
Sample
Sample Amount

Selected Column(s) Properties

☐ Show Value Units
☐ Use Default Font

Font...

OK Cancel

Summary Columns Setup

Common Summary

Table Properties

☐ Hide Value Units

Hide Columns

Start Time [min]
End Time [min]
Apex Value
Start Value
Start Value (Signal)
End Value
End Value (Signal)
Area [mV.s]
Height
Area [%]
Height [%]
W05 [min]
RB
Reten. Index [-]
Centroid [min]
Variance [min²]
Skew [-]
Excess 1-1

Show All
Show
Hide
Hide All

Show Columns

Reten. Time [min]
Response
Amount
Amount% [%]
Peak Type
Compound Name

User Columns

Add...
Edit Selected
Delete Selected

Selected Column(s) Properties

☐ Show Value Units
☐ Use Default Font

Font...

Preview

OK Cancel Default Help

CHROMATOGRAM WINDOW

SUMMARY TABLE OPTIONS

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

Summary Table

		Sample ID	Sample	Sample Amount	Reten. Time [min]	Response	Chloroform		Peak Type	Compound Name
							Amount	Amount%		
Data\Sample_Vial_6-	Signal 1	Halocarbons	Sample	0.000	3.660	61.116			IS	Chloroform
Data\Sample_Vial_6-	Signal 1	Halocarbons	Sample	0.000	3.667	62.733			IS	Chloroform
Data\Sample_Vial_7-	Signal 1	Halocarbons	Sample	0.000	3.680	271.936			IS	Chloroform
Data\Sample_Vial_7-	Signal 1	Halocarbons	Sample	0.000	3.673	268.931			IS	Chloroform

Results All Signals Results Summary Performance Integration Measurement Conditions SST Results

- Select All
- Copy
- Paste
- Summary Options...
- Restore Default Columns
- Setup Columns...
- User Columns
- Hide Column(s)
- Show Hidden Column(s)

Summary Table Options

☒ Table Inverted

☐ Show All Signals

Chromatogram Header

☒ Chromatogram / Signal

☐ Signal / Chromatogram

Summary Table

	Data\Sample_Vial_6-	Data\Sample_Vial_6-	Data\Sample_Vial_7-	Data\Sample_Vial_7-
	Signal 1	Signal 1	Signal 1	Signal 1
Sample ID	Halocarbons	Halocarbons	Halocarbons	Halocarbons
Sample	Sample	Sample	Sample	Sample
Sample Amount	0.000	0.000	0.000	0.000
Reten. Time [min]	3.660	3.667	3.680	3.673
Response	61.116	62.733	271.936	268.931
Amount [ul]	1.233	1.203	4.957	5.133
Amount% [%]	14.2	14.2	14.7	14.6
Peak Type	Ordnr (by ISTD 1)	Ordnr (by ISTD 1)	Ordnr (by ISTD 1)	Ordnr (by ISTD 1)
Compound Name	Chloroform	Chloroform	Chloroform	Chloroform
Reten. Time [min]	3.993	4.000	4.017	4.010
Response	183.931	188.187	806.060	800.418
Amount [ul]	1.210	1.176	4.791	4.981
Amount% [%]	13.9	13.9	14.2	14.2
Peak Type	Ordnr (by ISTD 1)	Ordnr (by ISTD 1)	Ordnr (by ISTD 1)	Ordnr (by ISTD 1)
Compound Name	Trichloroethane	Trichloroethane	Trichloroethane	Trichloroethane

Results All Signals Results Summary Performance Integration Measurement Conditions SST Results

Summary Table Options

☐ Table Inverted

☐ Show All Signals

Chromatogram Header

☒ Chromatogram / Signal

☐ Signal / Chromatogram

Report in Summary Table

☒ All Identified Peaks

☐ All Peaks in Calibration

Parameter Header

☒ Compound / Parameter

☐ Parameter / Compound

Summary Table

		Sample ID	Sample	Sample Amount	Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
Data\Sample_Vial_6-	Signal 1	Halocarbons	Sample	0.000	3.660	61.116	1.233	14.2	Ordnr (by IS	Chloroform
Data\Sample_Vial_6-	Signal 1	Halocarbons	Sample	0.000	3.667	62.733	1.203	14.2	Ordnr (by IS	Chloroform
Data\Sample_Vial_7-	Signal 1	Halocarbons	Sample	0.000	3.680	271.936	4.957	14.7	Ordnr (by IS	Chloroform
Data\Sample_Vial_7-	Signal 1	Halocarbons	Sample	0.000	3.673	268.931	5.133	14.6	Ordnr (by IS	Chloroform

Summary Table Options

☐ Table Inverted

☐ Show All Signals

Chromatogram Header

☒ Chromatogram / Signal

☐ Signal / Chromatogram

Report in Summary Table

☒ All Identified Peaks

☐ All Peaks in Calibration

Parameter Header

☐ Compound / Parameter

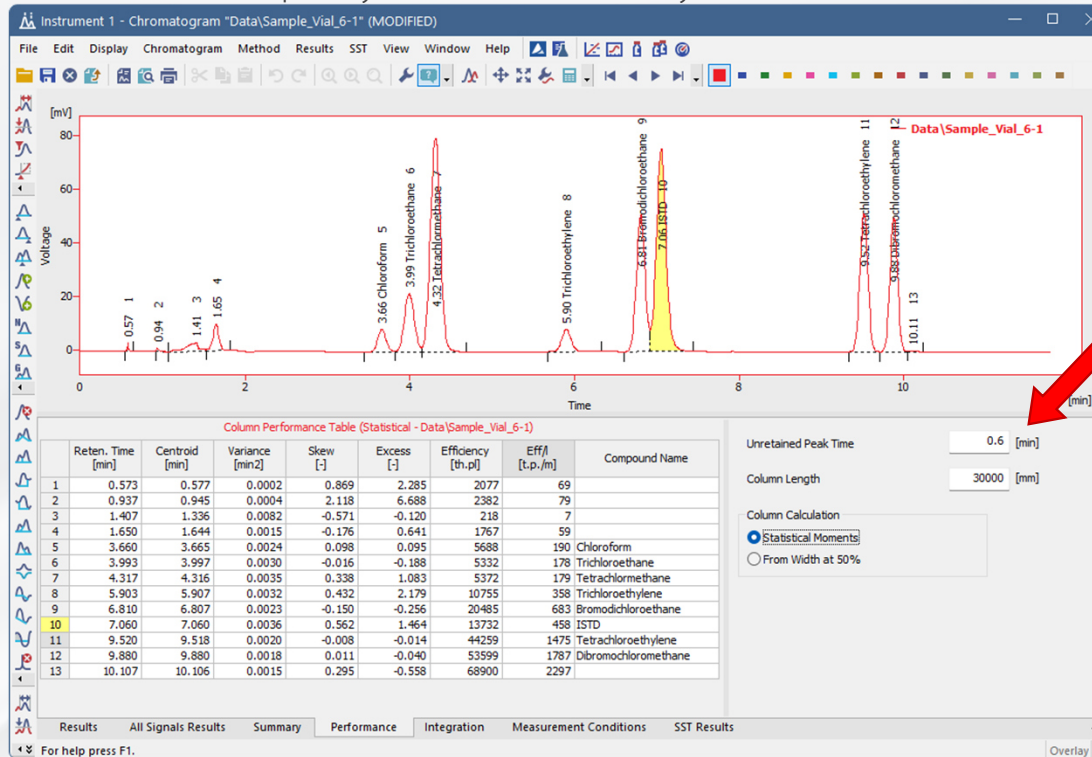
☒ Parameter / Compound

Summary Table												
		Sample ID	Sample	Sample Amount	Reten. Time [min]							
					Chloroform	Trichloroethane	Tetrachloroethane	Trichloroethylene	Bromodichloroethane	ISTD	Tetrachloroethylene	Dibromomethane
Data\Sample_Vial_6-	Signal 1	Halocarbons	Sample	0.000	3.660	3.993	4.317	5.903	6.810	7.060	9.520	
Data\Sample_Vial_6-	Signal 1	Halocarbons	Sample	0.000	3.667	4.000	4.320	5.910	6.817	7.060	9.527	
Data\Sample_Vial_7-	Signal 1	Halocarbons	Sample	0.000	3.680	4.017	4.340	5.910	6.827	7.060	9.530	
Data\Sample_Vial_7-	Signal 1	Halocarbons	Sample	0.000	3.673	4.010	4.337	5.907	6.820	7.063	9.527	

CHROMATOGRAM WINDOW

PERFORMANCE TABLE

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



Method Setup Demo1 - #4; 11/13/2023 2:20:03 PM

New Open... Save Save as... Report setup... Audit trail... Send method by e-mail... Help

Common for all detectors

Subtraction
Chromatogram: [None]
Matching: No Change
Set... None

Column Calculations
Unretained Time: 0.6 [min]
Column Length: 30000 [mm]
☒ Statistical Moments
☐ From Width at 50%

Auxiliary Signal Store

User Variables
Variable 1: Name MethodUserVar1, Value 0
Variable 2: Name MethodUserVar2, Value 0
Variable 3: Name MethodUserVar3, Value 0

Event Table Measurement Acquisition Integration Calculation Advanced

OK Cancel Send Method

CHROMATOGRAM WINDOW

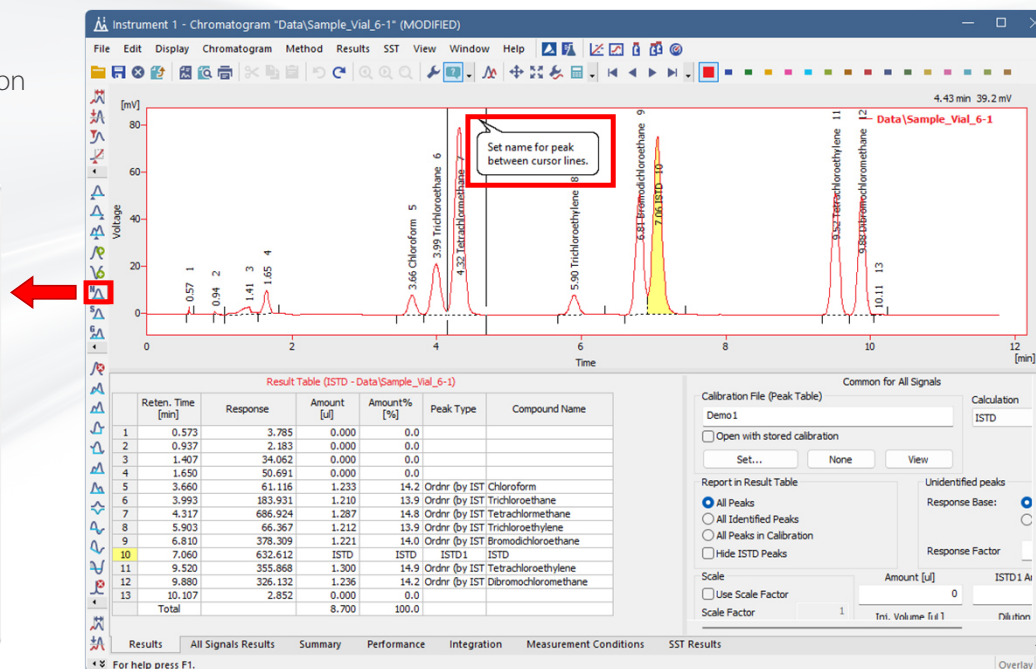
FORCE PEAK NAME

- Set compound from calibration
- Set custom name

Peak - Force Peak Name

Bromodichloroethane
 Chloroform
 Dibromochloromethane
 ISTD
 Tetrachloromethane
 Tetrachloroethylene
 Trichloroethane
 Trichloroethylene

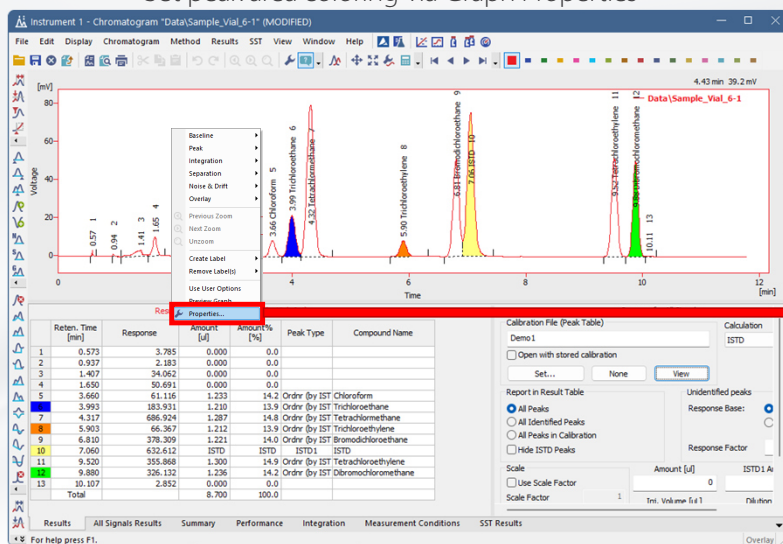
OK Cancel Help



CHROMATOGRAM WINDOW

PEAK COLORS

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



Instrument 1 - Calibration Calib\Demo1 <-- ISTD (MODIFIED)

Calibration Summary Table (ISTD - Calib\Demo1 - Signal 1)

Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color
1	Chloroform	3.717	0.200 min	0.200 min	Ordrr		None	ISTD	Blue
2	Trichloroethane	4.053	0.200 min	0.200 min	Ordrr		None	ISTD	Orange
3	Tetrachloromethane	4.387	0.200 min	0.200 min	Ordrr		None	ISTD	Yellow
4	Trichloroethylene	5.960	0.200 min	0.200 min	Ordrr		None	ISTD	Green
5	Bromodichloroethane	6.870	0.200 min	0.200 min	Ordrr		None	ISTD	Blue
6	ISTD	7.107	0.200 min	0.200 min	Ordrr		ISTD1	ISTD	Blue
7	Tetrachloroethylene	9.567	0.200 min	0.200 min	Ordrr		None	ISTD	Blue
8	Dibromochloromethane	9.930	0.200 min	0.200 min	Ordrr		None	ISTD	Blue

Compounds: Chloroform Trichloroethane Tetrachloromethane Trichloroethylene Bromodichloroethane ISTD

For help press F1.

Graph Properties

Graph Axes Appearance Time Axis Signal Axis Signals Gradient & Auxiliary Signals Auxiliary Signal Details

☐ Use User Options
☐ Preview Graph
☐ Show Workplace Labels
☐ Show Grid
☐ Show Legend
☐ Show Balloon Help
☐ Show Events
☐ Show Data Points

Baseline
☒ Line
☐ Marks

Color:
☐ As Active Signal
☐ As Active Signal

Peak Tags
☒ Simplified Peak Tags
☒ Retention Time
☒ Name
☒ Peak Number
☒ Group ID

Enhanced Format...

Font...

Border:
☐ Windows Default
☐ Select...

Background Colors
☒ Windows Default
☐ Select...

Report in Result Table
☒ All Peaks
☐ All Identified Peaks
☐ All Peaks in Calibration
☐ Hide ISTD Peaks

Response Base:
☐ Response Factor
☐ Amount [µl]
☐ ISTD1 A

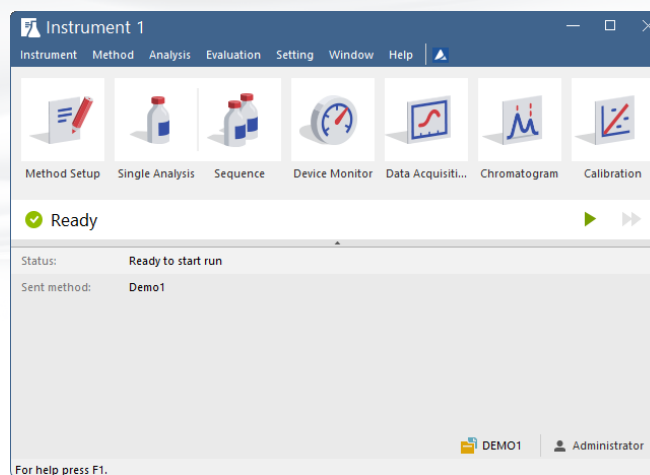
Scale
☐ Use Scale Factor
☐ Scale Factor 1
☐ Int. Volume (µl) 1
☐ Unit

Peak Area Coloring
☒ Set by Calibration
☐ Highlight Selected Peaks in Graph

OK Cancel Apply Help

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

Instrument 1 - Calibration Calib\ASTM6730_CS-C15-R1 -< ESTD (MODIFIED)																			
File Edit Display Calibration View Window Help																			
Automatic Calibration on All Signals																			
Calibration Summary Table (ESTD - Calib\ASTM6730_CS-C15-R1 - Signal 1)																			
Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	Reten. Index	LOD	LOQ	Response Base	Manual Resp. Factor	Response	Amount	Resp. Fact.	Rec No.	
1	n-Pentane	12.857	0.200 min	0.200 min	Ordrr	None	None			500.000	0.000	0.000		0.0000	4724.4275	0.000	0.0000	1/1	
2	n-Hexane	20.500	0.200 min	0.200 min	Ordrr	None	None			600.000	0.000	0.000		0.0000	4384.6177	0.000	0.0000	1/1	
3	n-Heptane	28.880	0.200 min	0.200 min	Ordrr	None	None			700.000	0.000	0.000		0.0000	8713.0309	0.000	0.0000	1/1	
4	n-Octane	38.693	0.200 min	0.200 min	Ordrr	None	None			800.000	0.000	0.300		0.0000	10596.7032	0.000	0.0000	1/1	
5	n-Nonane	49.687	0.200 min	0.200 min	Ordrr	None	None			900.000	0.000	0.300		0.0000	11577.5428	0.000	0.0000	1/1	
6	n-Decane	61.063	0.200 min	0.200 min	Ordrr	None	None			1000.000	0.000	0.300		0.0000	6271.1765	0.000	0.0000	1/1	
7	n-Undecane	72.393	0.200 min	0.200 min	Ordrr	None	None			1100.000	0.100	0.300		0.0000	12734.3308	0.000	0.0000	1/1	
8	n-Dodecane	83.017	0.200 min	0.200 min	Ordrr	None	None			1200.000	0.100	0.300		0.0000	6416.3005	0.000	0.0000	1/1	
9	n-Tridecane	93.273	0.200 min	0.200 min	Ordrr	None	None			1300.000	0.100	0.300		0.0000	13119.1941	0.000	0.0000	1/1	
10	n-Tetradecane	102.720	0.200 min	0.200 min	Ordrr	None	None			1400.000	0.100	0.300		0.0000	6801.6947	0.000	0.0000	1/1	
11	n-Pentadecane	111.883	0.200 min	0.200 min	Ordrr	None	None			1500.000	0.100	0.300		0.0000	14341.0531	0.000	0.0000	1/1	
Compounds n-Pentane n-Hexane n-Heptane n-Octane n-Nonane n-Decane n-Undecane n-Dodecane																			
For help press F1.																			

Instrument 1 - Chromatogram "Data\N_PARAFFINS_FOR_ASTM6730 - Detector A" - #12; 20/04/2023 23:08:18

File Edit Display Chromatogram Method Results SST View Window Help

Result Table (ESTD - Data\N_PARAFFINS_FOR_ASTM6730 - Detector A)

Reten. Time [min]	Response	Amount [mg]	Amount [%]	Peak Type	Compound Name
1	12.803	2288.743	0.000	Ordrr Free	n-Pentane
2	20.430	3449.147	0.000	Ordrr Free	n-Hexane
3	28.863	6432.241	0.000	Ordrr Free	n-Heptane
4	38.673	7015.205	0.000	< LOQ Ordrr	n-Octane
5	49.657	7091.212	0.000	< LOQ Ordrr	n-Nonane
6	61.087	7541.664	0.000	< LOQ Ordrr	n-Decane
7	72.323	7397.085	0.000	< LOQ Ordrr	n-Undecane
8	83.057	7835.542	0.000	< LOQ Ordrr	n-Dodecane
9	93.147	6239.622	0.000	< LOQ Ordrr	n-Tridecane
10	102.747	8052.391	0.000	< LOQ Ordrr	n-Tetradecane
11	111.750	7469.893	0.000	< LOQ Ordrr	n-Pentadecane
Total			0.000		

Results All Signals Results Summary Performance Integration Measurement Conditions SST Results

For help press F1.

Common for All Signals

Calibration File (Peak Table)
ASTM6730_CS-C15-R1

Calculation
ESTD

☐ Open with stored calibration

Set... None View

Report in Result Table

☒ All Peaks
☐ All Identified Peaks
☐ All Peaks in Calibration
☐ Hide ISTD Peaks

Unidentified peaks

Response Base: ☒ Area
☐ Height

Response Factor

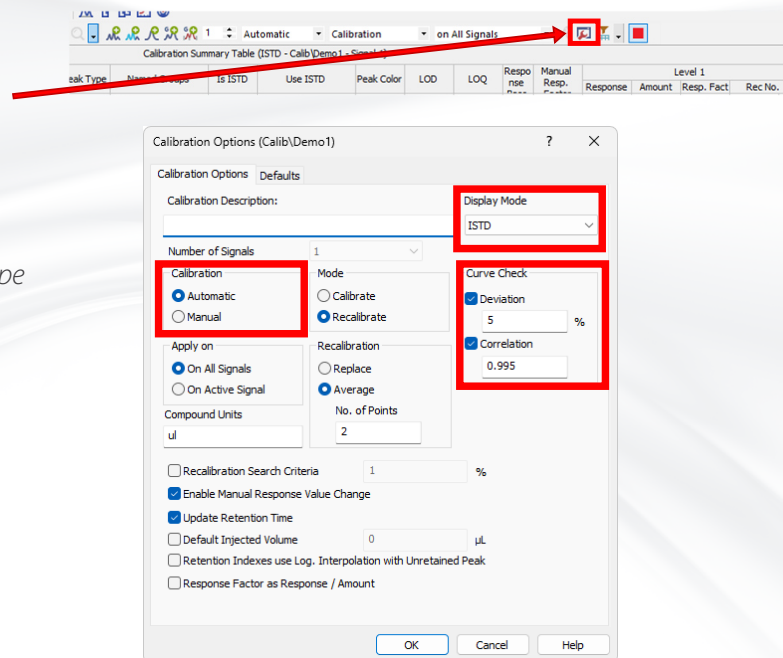
Grade Amount Found

Overlay

CALIBRATION

CALIBRATION OPTIONS

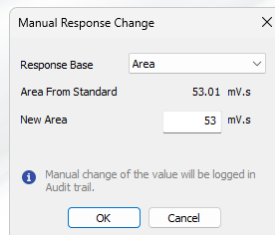
- Open via *Calibration – Options* or Calibration Options button
- Display Mode – related to calculation types: ESTD, ISTD, NORM, STDADD
- Calibration curve check – threshold used for the **Failure** message in *Result Table – Peak Type*
- Automatic/Manual calibration



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



Manual Response Change

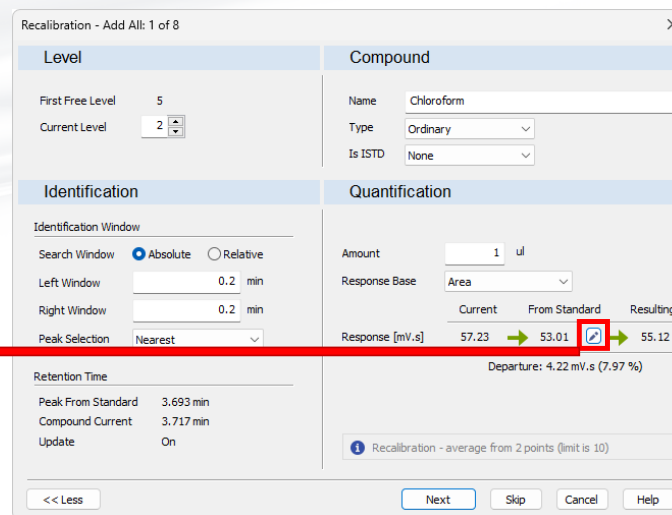
Response Base: Area

Area From Standard: 53.01 mV.s

New Area: 53 mV.s

Manual change of the value will be logged in Audit trail.

OK Cancel



Recalibration - Add All: 1 of 8

Level	Compound
First Free Level: 5 Current Level: 2	Name: Chloroform Type: Ordinary Is ISTD: None
Identification	Quantification
Identification Window Search Window: <input checked="" type="radio"/> Absolute <input type="radio"/> Relative Left Window: 0.2 min Right Window: 0.2 min Peak Selection: Nearest	Amount: 1 ul Response Base: Area Current: 57.23 From Standard: 53.01 Resulting: 55.12 Departure: 4.22 mV.s (7.97 %)
Retention Time Peak From Standard: 3.693 min Compound Current: 3.717 min Update: On	Recalibration - average from 2 points (limit is 10)

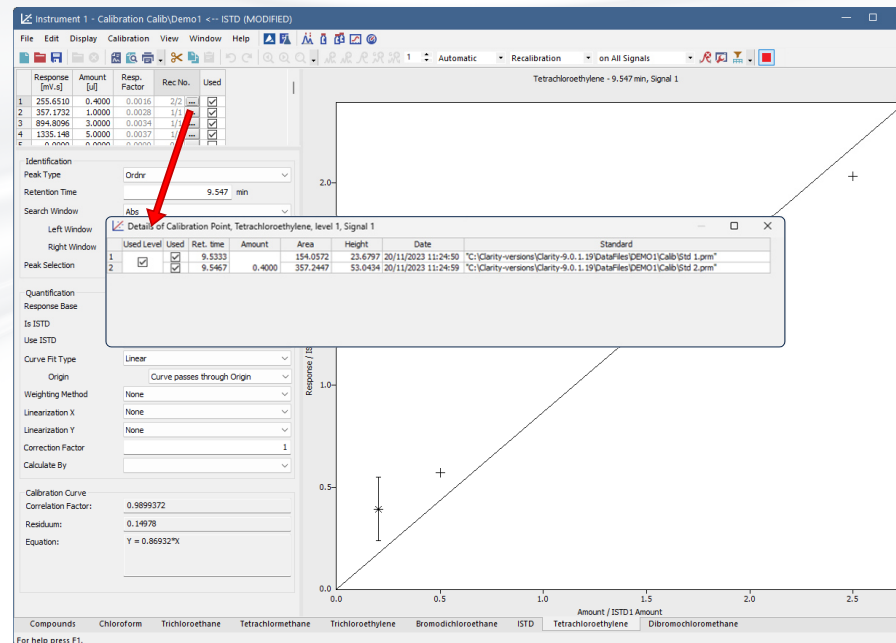
<< Less Next Skip Cancel Help



CALIBRATION

DETAILS OF CALIBRATION POINT

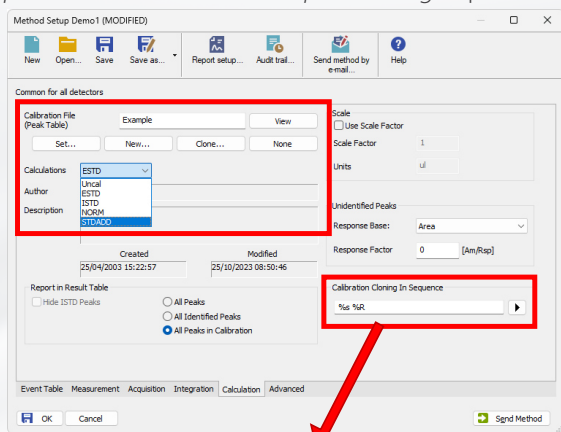
- When recalibrating a level using more points, you can view calibration point details for selected level (accessible also via *Calibration – Show Details*)
- Checkbox state – include/omit from calibration



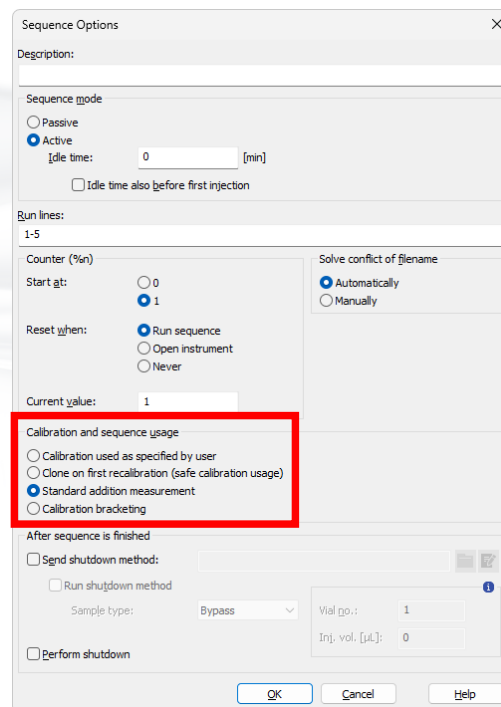
CALIBRATION

BRACKETING AND STANDARD ADDITION

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



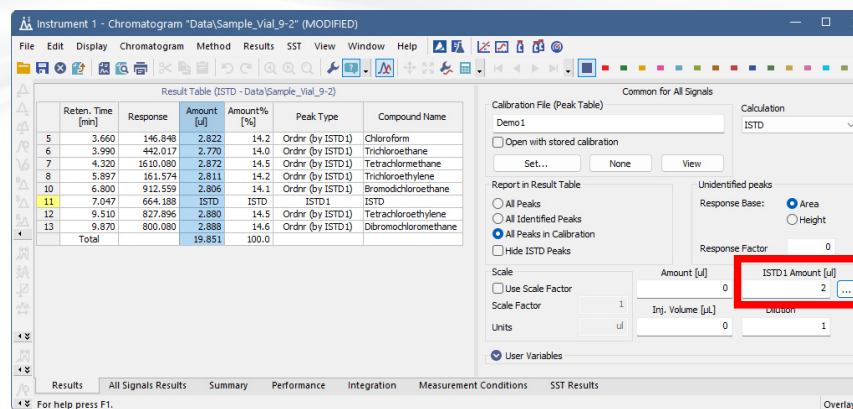
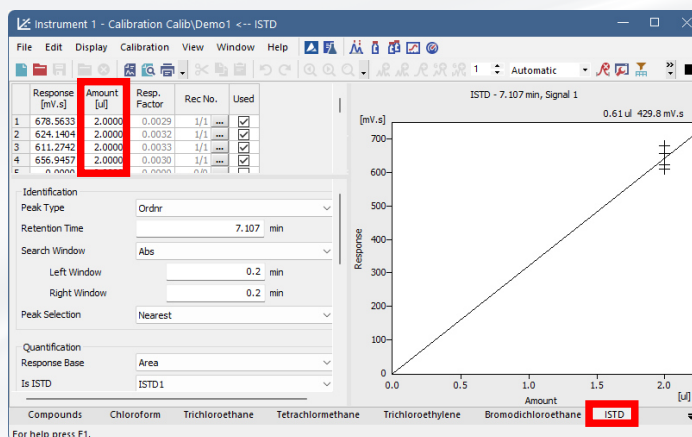
- Name of calibration clone used if the method selected in *Calibration and sequence usage* supports cloning



CALCULATIONS

ISTD

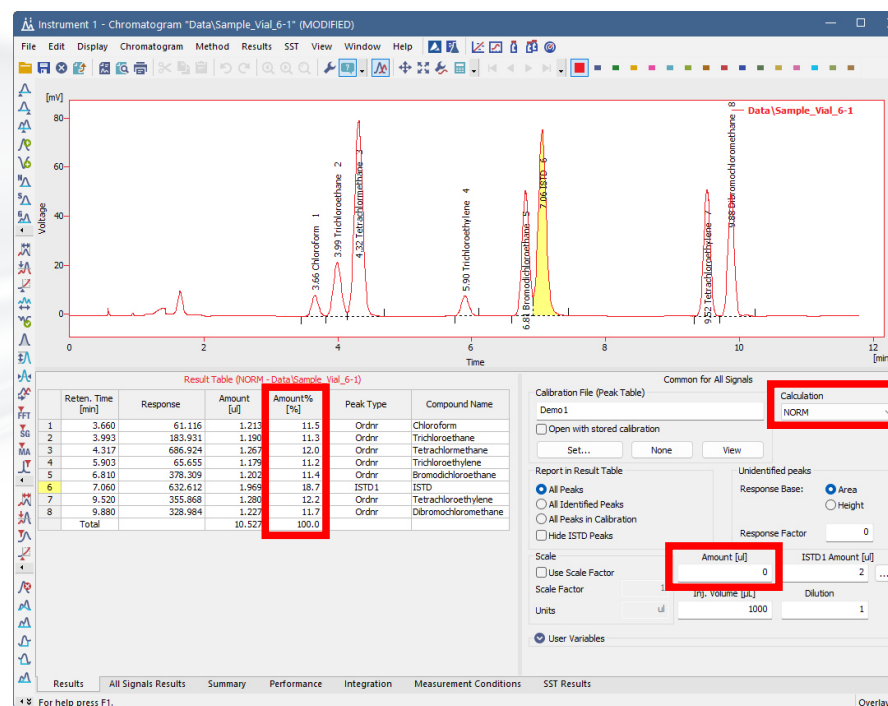
- Up to ten ISTD compounds can be present in the calibration/sample
- 2 types of ISTD calculations available:
 - Any amount of ISTD (both calibration and sample chromatogram contain the used ISTD amount)
 - Same amount of ISTD in samples and standards (ISTD amount = 0 in **both** locations)



CALCULATIONS

NORMALIZED %

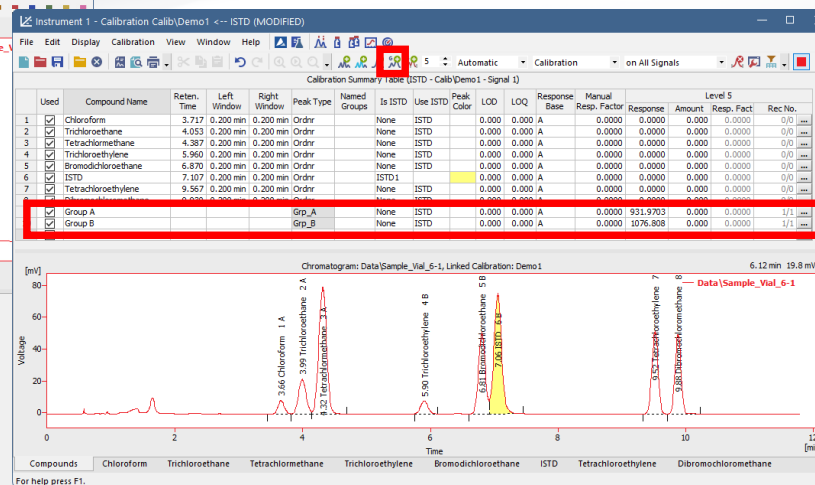
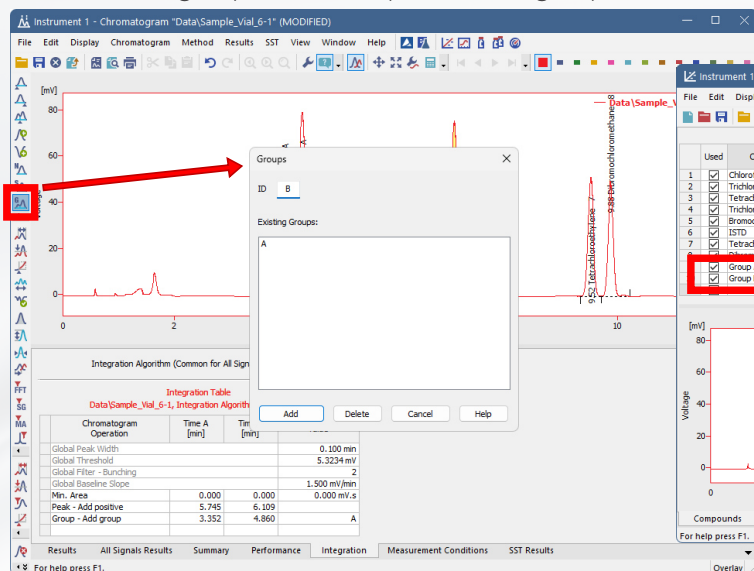
- Amount % column contains the normalized percentage **if all integrated peaks are calibrated**
- If the Sample Amount is 0, compounds in the Amount % column add up to a total of 100%
- Otherwise, the value serves as the total sum of Amount %, and values in the Amount % column are normalized to the Amount 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



23.0331



Clarity™

ADVANCED CHROMATOGRAPHY SOFTWARE



SHORT BREAK