

23.0331



Clarity™

ADVANCED CHROMATOGRAPHY SOFTWARE

CLARITY TRAINING

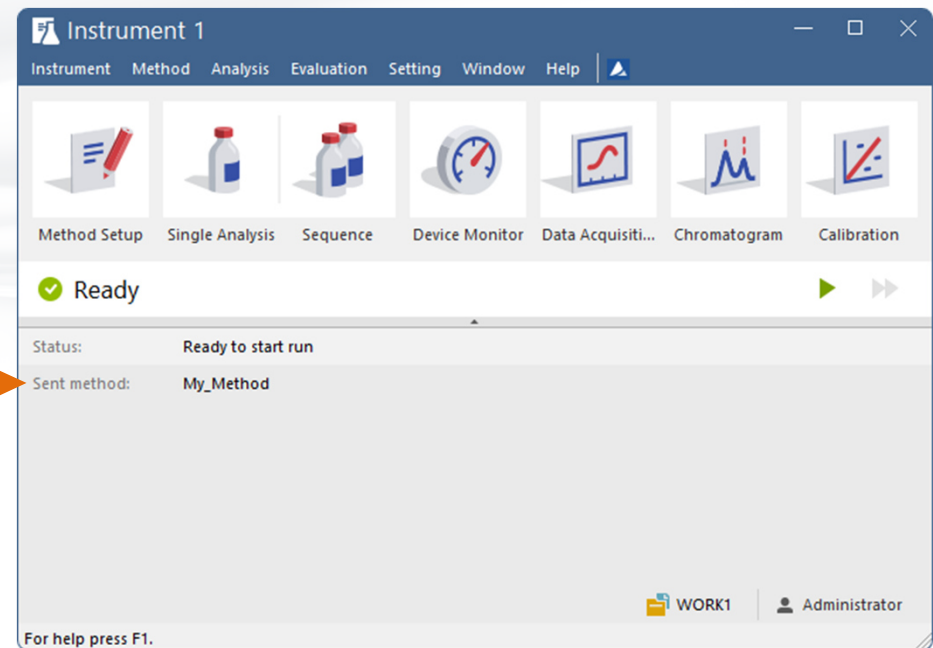
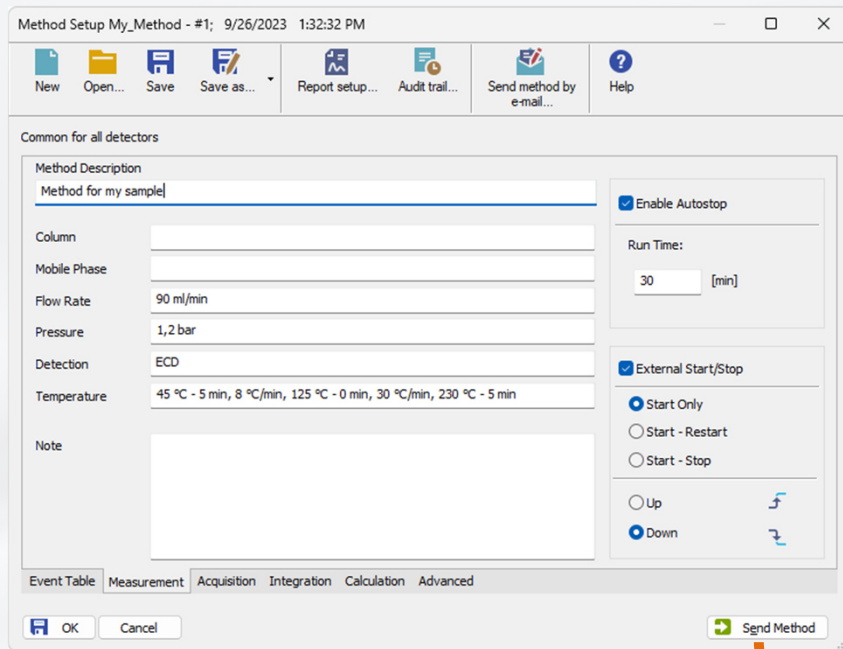
BASIC OPERATIONS

CONTENT

- Developing a method
- Acquiring data
 - Single Analysis
 - Sequence
- Creating calibration
- Reporting results

METHOD IN CLARITY

- > Instrumental and processing parameters within one document
- > Can be sent to HW directly from Method Setup
- > Stored as *.met file in current project folder



METHOD DEVELOPMENT

PROPOSED WORKFLOW

- Set acquisition parameters
- Enter sample information (optional)
- Acquire the first chromatogram
- Optimize integration parameters
- Store the method for further analyses

METHOD DEVELOPMENT

METHOD SETUP

Method Setup Default1 - #5: 10.12.2024 13:41:11

Time [min]	A [%]	B [%]	C [%]	D [%]	Flow [mL/min]
1	Initial	0,0	0,0	0,0	100,0
2	0,50	0,0	30,0	0,0	70,0
3	1,00	30,0	30,0	40,0	0,0
4					10,000

Method Setup Default1 - #6: 10.12.2024 13:45:14

Select GC: GC 1 (Enabled)

Oven Valve: External LPC Log

Mode: Isothermal

Run Time [min]: 10,0

Configuration: Init. Temp [°C]: 50 Off; Init. Time [min]: 10

Setup: Max. Temp [°C]: 450; Equ. Time [min]: 1

Auto Run Start: Auto Run Start; Post Run

Repeat #: 0; Temp [°C]: 0

Cycle Time [min]: 0; Time [min]: 0

Instrument 1: Ready

Status: Ready to start run

Sent method: My_Method

- Accessed from Instrument window
- Available tabs are dependent on used configuration

METHOD SETUP

MEASUREMENT TAB

- > Description
 - Informative
- > Autostop & Run time
- > External Start/Stop

Method Setup Ethanol in blood - #3; 9/26/2023 2:03:37 PM

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

Common for all detectors

Method Description
DEMO Example - GC - Autosampler - Ethanol in blood

Column db 624-30m-3.0u-0,32 id

Mobile Phase hydrogen

Flow Rate 50 cm/min

Pressure 5.57 psi

Detection FID

Temperature Ramped to 225

Note short linear velocity 50 cm/sec
column initial 45 deg

Enable Autostop

Run Time:
4 [min]

External Start/Stop

Start Only
 Start - Restart
 Start - Stop

Up
 Down

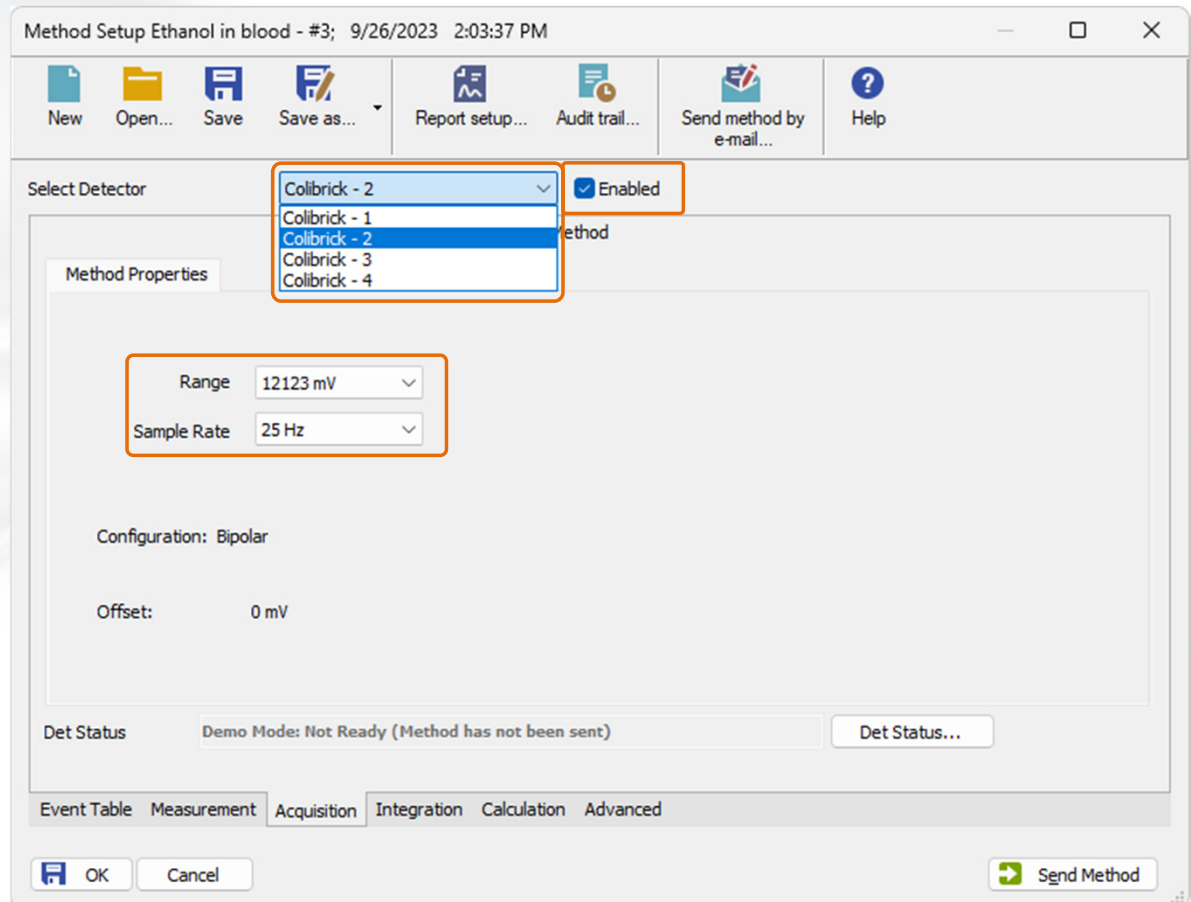
Event Table Measurement Acquisition Integration Calculation Advanced

OK Cancel Send Method

METHOD SETUP

ACQUISITION TAB

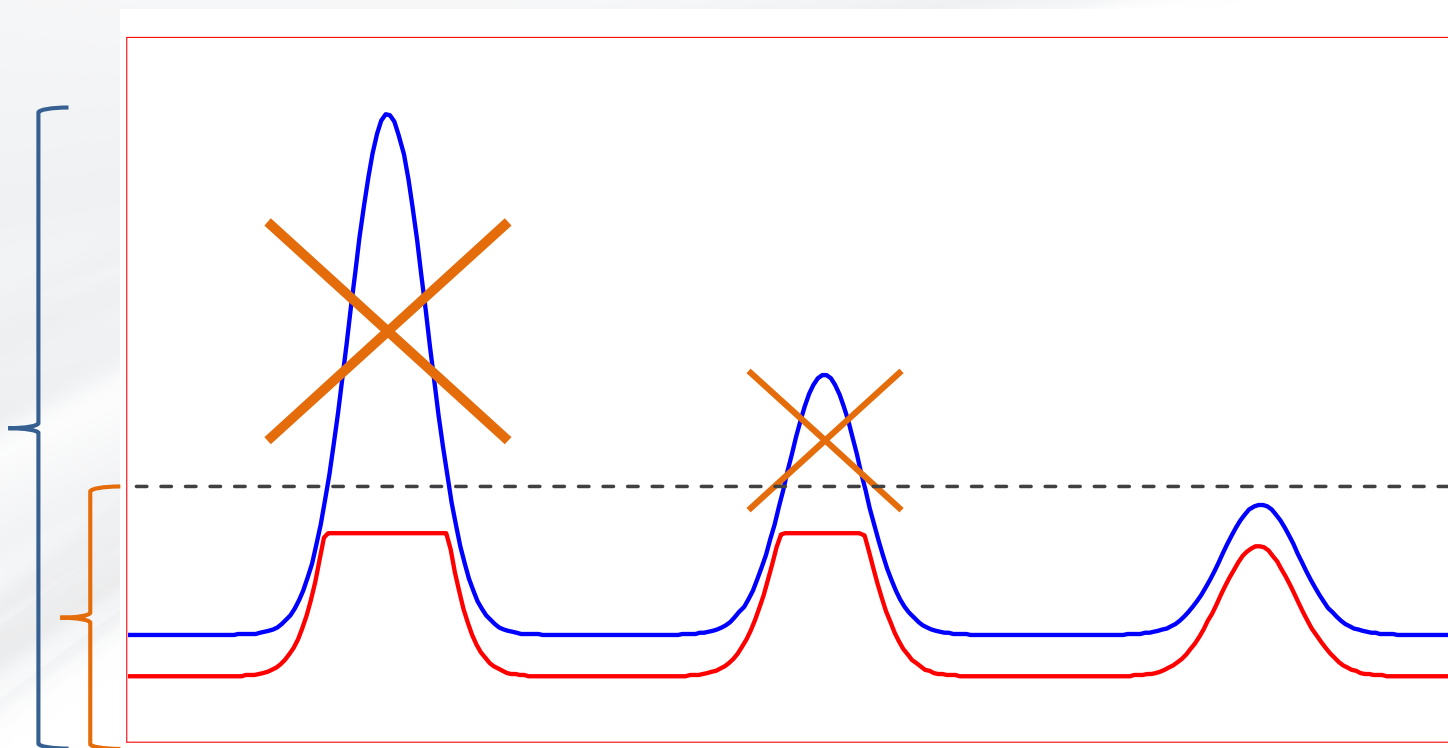
- > Device-specific
- > **Cannot** be modified during acquisition
- > "Enabled" checkbox



METHOD SETUP

SIGNAL RANGE

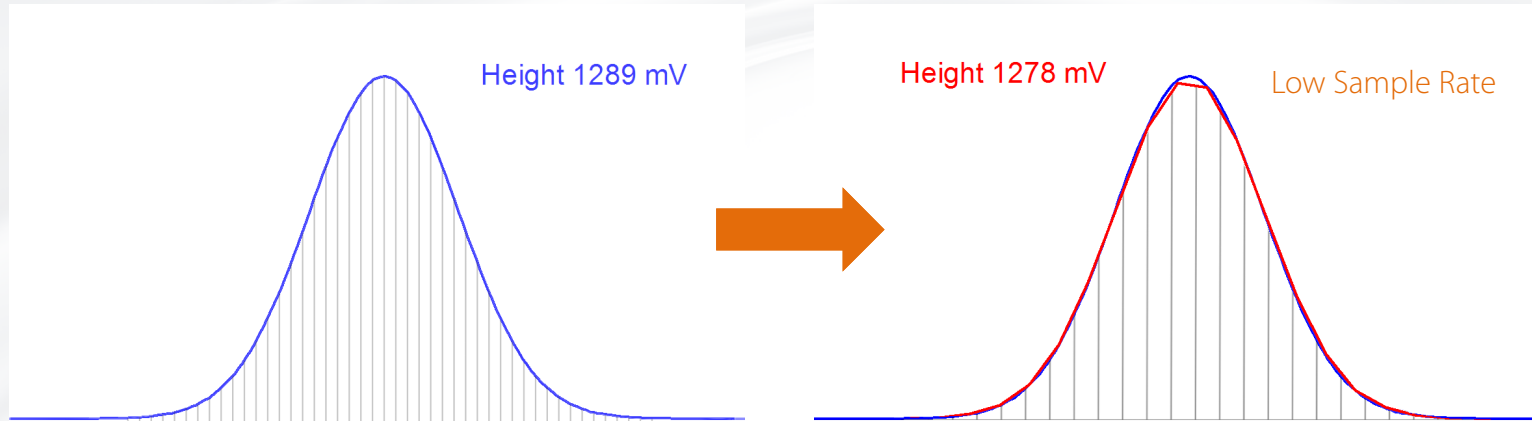
- Signal out of range = loss of information



METHOD SETUP

SAMPLE RATE

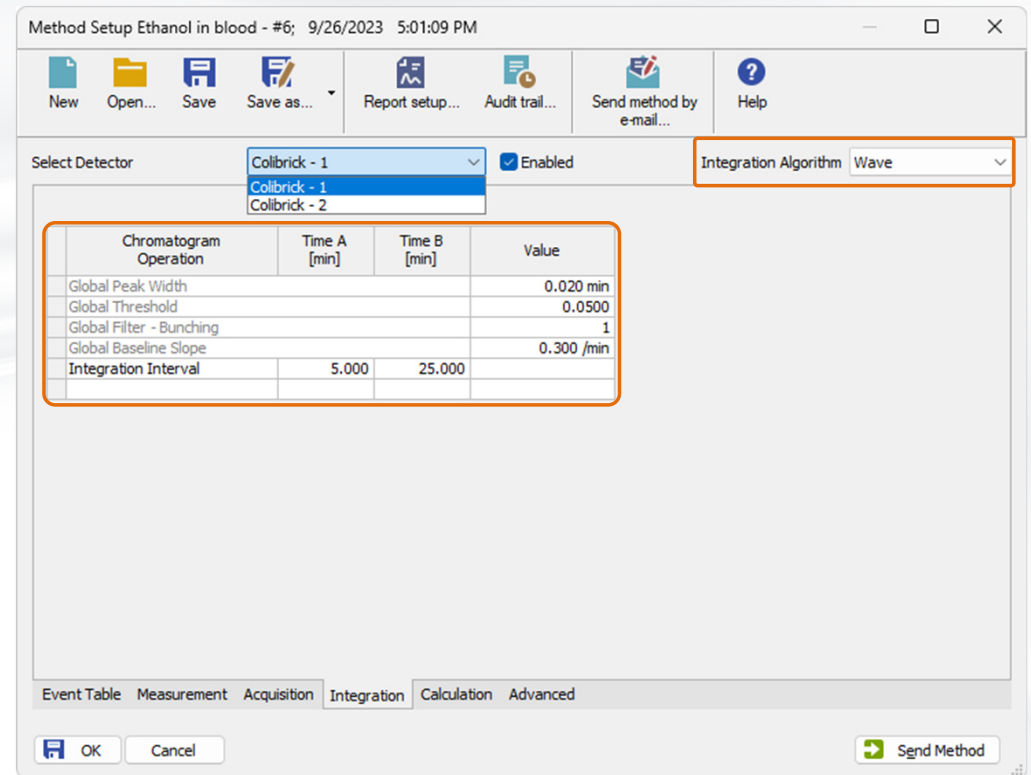
- Too low = not enough datapoints per peak = incorrect results
- “Correct” rate is dependent on HW and analytical application
 - GC detectors – usually 25-50 Hz
 - LC and Spectral detectors – according to application and HW parameters



METHOD SETUP

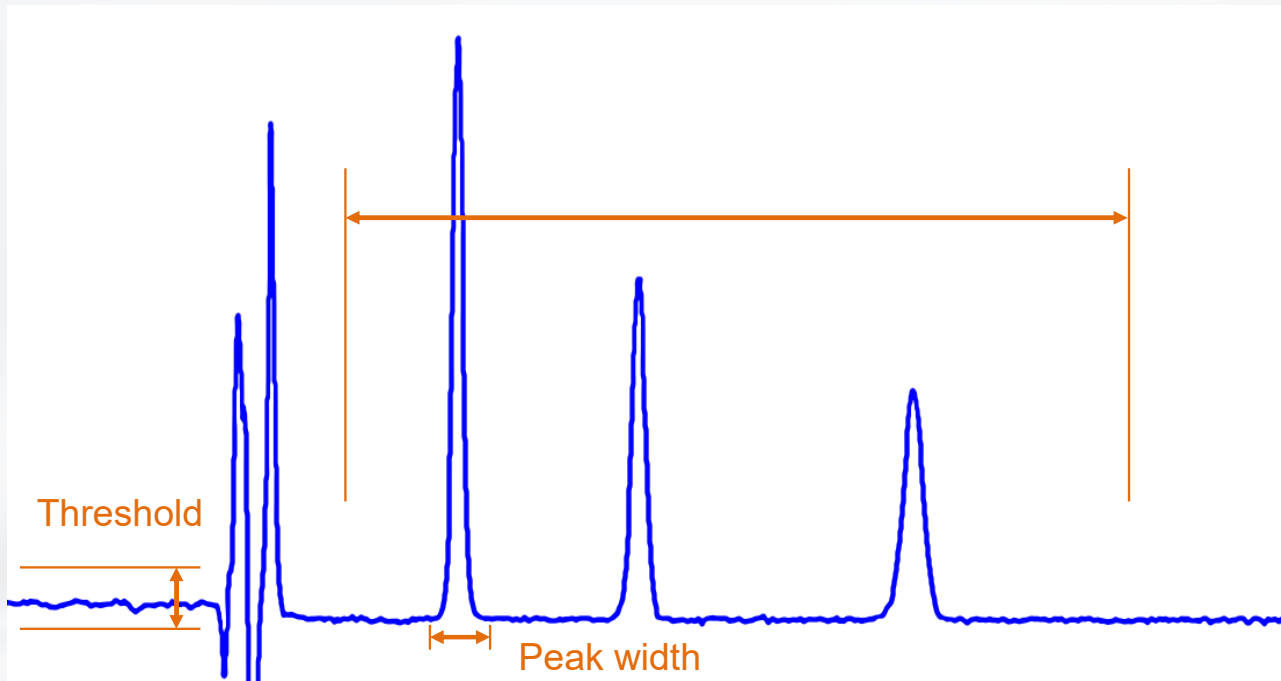
INTEGRATION TAB

- > Parameters are applied to measured chromatograms
- > Integration table is separate for each signal
- > Selection of integration algorithm



METHOD SETUP

INTEGRATION PARAMETERS

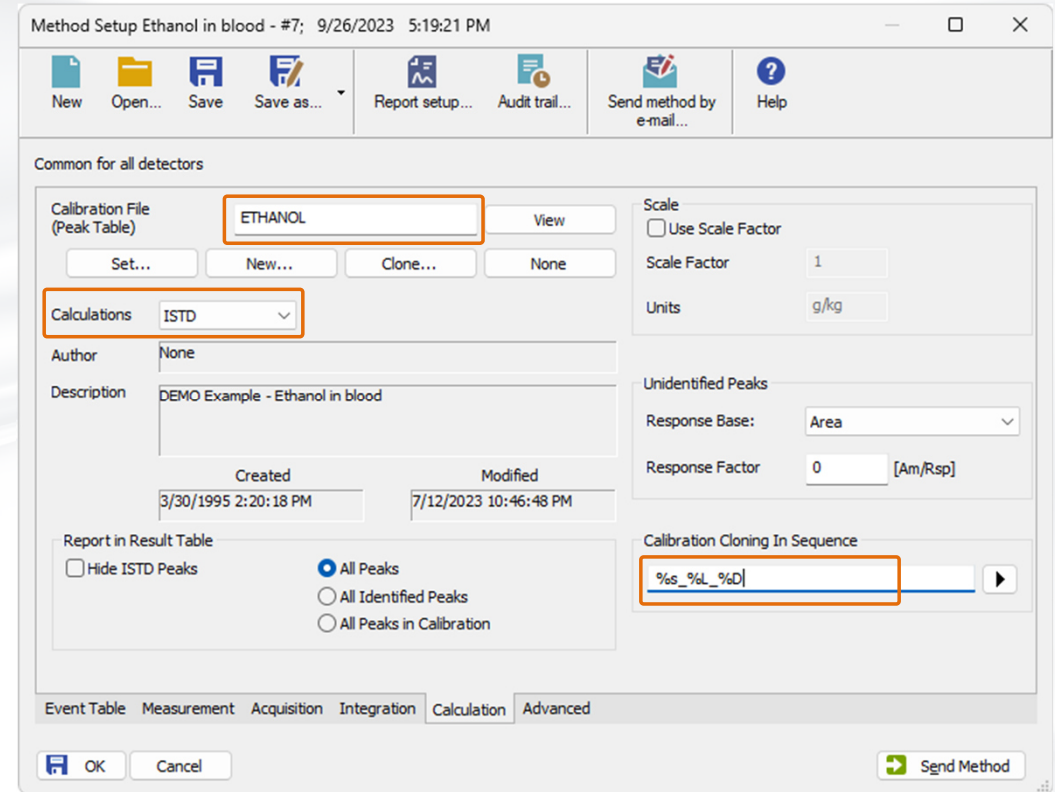


- > Global parameters
 - Peak width, Threshold, Bunching, Slope
- > Integration Interval
- > Other interval and peak functions

METHOD SETUP

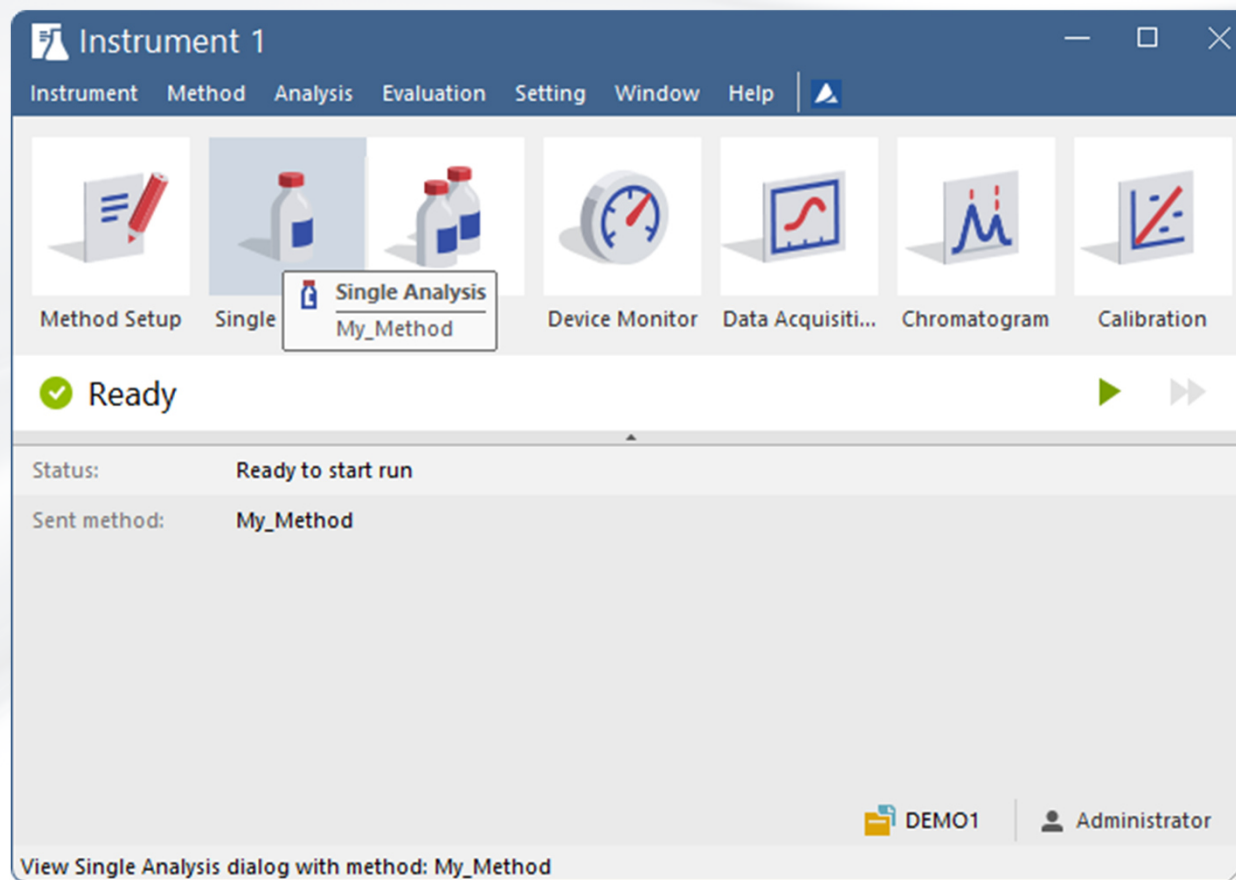
CALCULATION TAB

- > Calibration that is linked to measured chromatograms
- > Calculation type
- > Calibration cloning



METHOD DEVELOPMENT

SINGLE ANALYSIS – FIRST RUN



SINGLE ANALYSIS

ANALYSIS TAB

- > Enter sample information
- > Enter file name
 - Use variables by clicking ▶

Single Analysis

Sample ID Batch-#95

Sample Sample-#02

Comments

Amount 0 ISTD1 Amount 500

Dilution 1 Inj. Volume [µL] 10

Sample Type Unknown Level 1

Method My_Method Edit Method...

Analysis Post Run Settings User Variables

Control

Send method Inject & Run Stop Abort Snapshot

Use Autosampler Vial 2

Chromatogram File Name (Data\Batch-#95_Sample-#02_My_Method_26_09_2023_1)

%q_%Q_%I_%D_%n

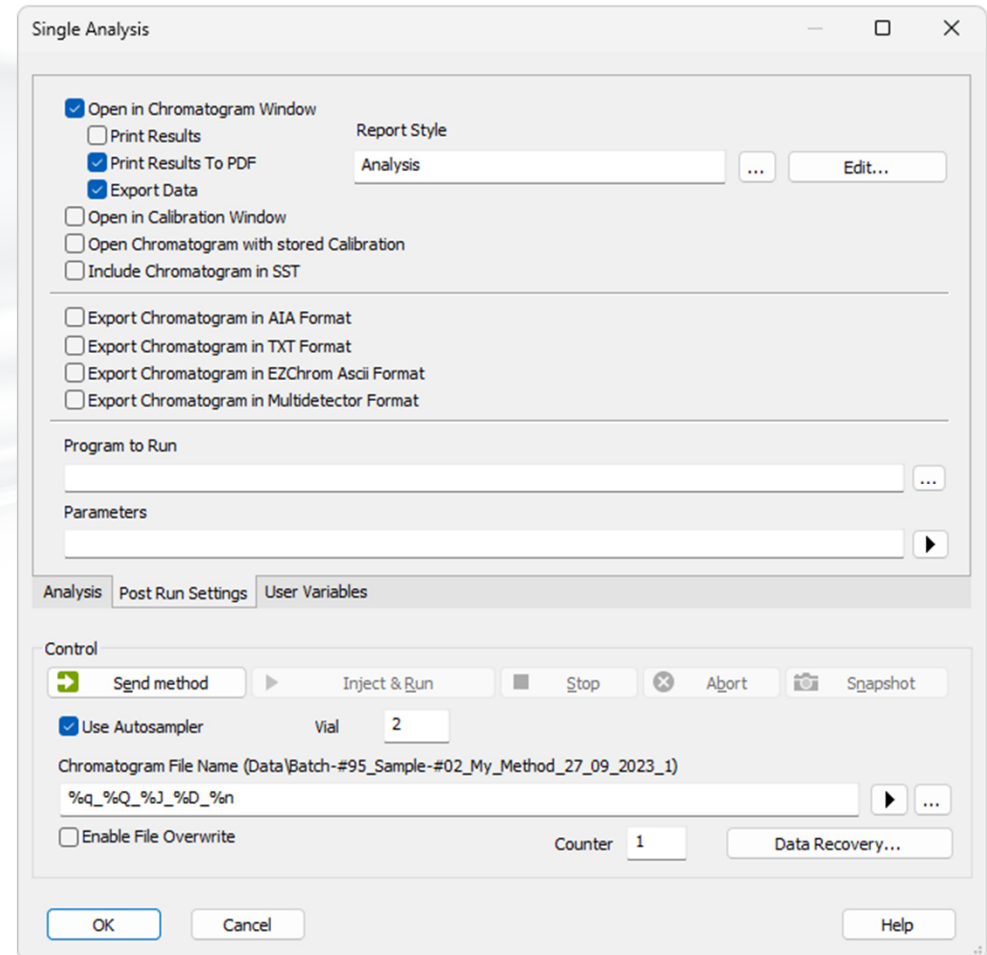
Enable File Overwrite Counter 1 Data Recovery...

OK Cancel Help

SINGLE ANALYSIS

POST RUN SETTINGS TAB

- Automatic operations after the end of analysis



SINGLE ANALYSIS

SENDING METHOD

Single Analysis

Sample ID: Batch-#95
Sample: Sample-#02
Comments: ...
Amount: 0 ISTD1 Amount: 500
Dilution: 1 Inj. Volume [µL]: 10
Sample Type: Unknown Level: 1
Method: My_Method Edit Method...

Analysis Post Run Settings User Variables

Control
Send method Inject & Run Stop Abort Snapshot
Use Autosampler Vial 2
Chromatogram File Name (Data)Batch-#95_Sample-#02_My_Method_26_09_2023_1
%q_%Q_%J_%D_%n
Enable File Overwrite Counter 1 Data Recovery...

OK Cancel Help



Single Analysis

Sample ID: Batch-#95
Sample: Sample-#02
Comments: ...
Amount: 0 ISTD1 Amount: 500
Dilution: 1 Inj. Volume [µL]: 10
Sample Type: Unknown Level: 1
Method: My_Method Edit Method...

Analysis Post Run Settings User Variables

Control
Send method Inject & Run Stop Abort Snapshot
Use Autosampler Vial 2
Chromatogram File Name (Data)Batch-#95_Sample-#02_My_Method_27_09_2023_1

Instrument 1
Instrument Method Analysis Evaluation Setting Window Help

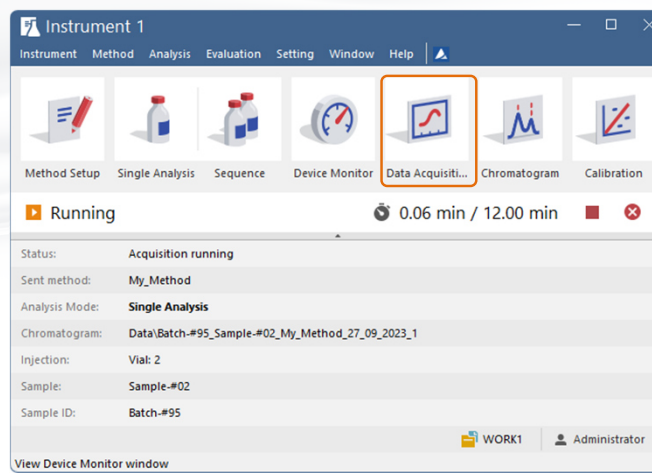
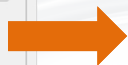
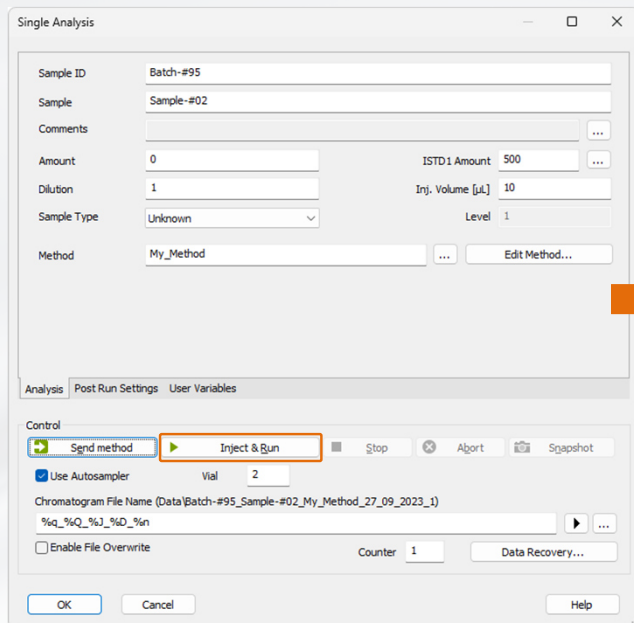
Method Setup Single Analysis Sequence Device Monitor Data Acquisiti... Chromatogram Calibration

Ready
Status: Ready to start run
Sent method: My_Method

WORK1 Administrator
For help press F1.

METHOD DEVELOPMENT

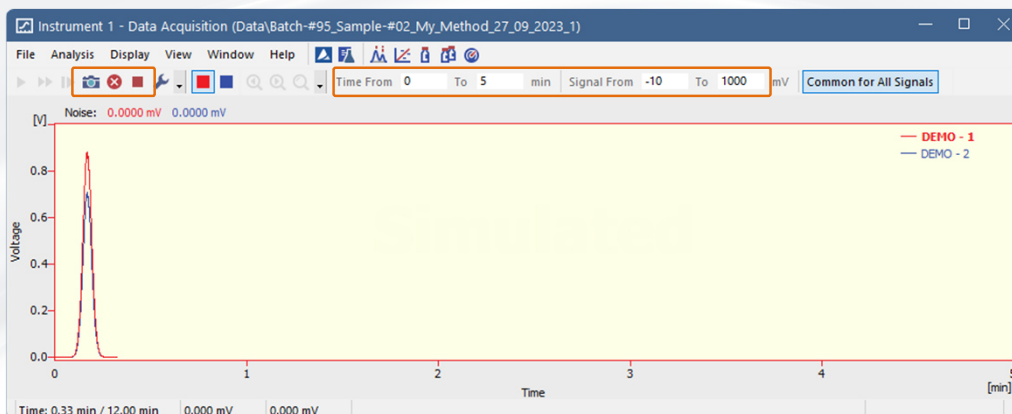
DATA ACQUISITION



DATA ACQUISITION

MONITORING ANALYSIS

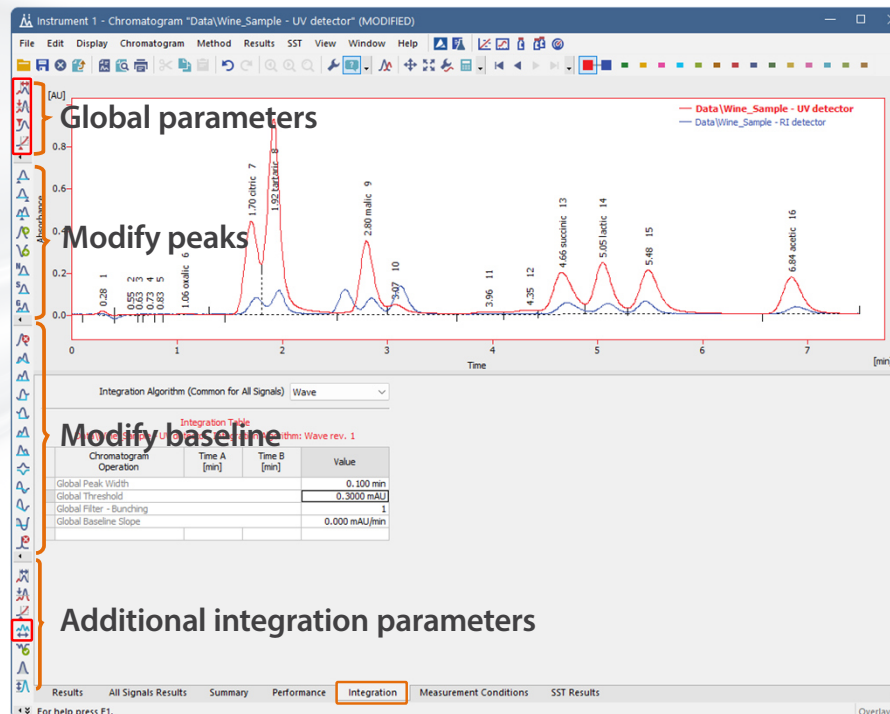
- > Functions
 - Snapshot – Temporary chromatogram
 - Abort – End analysis, no chromatogram saved
 - Stop – End analysis, save chromatogram
- > Parameters – Only influence view, not data itself



METHOD DEVELOPMENT

FIRST CHROMATOGRAM

- > Optimize integration
 - Global parameters
 - Integration interval
 - Other functions
- > Change integration algorithm

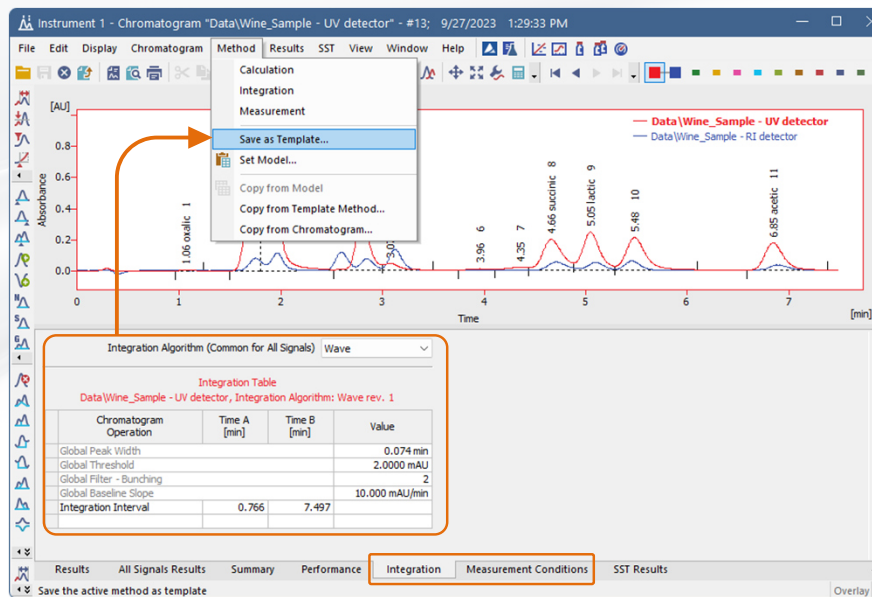


CHROMATOGRAM

SAVING OPTIMIZED METHOD

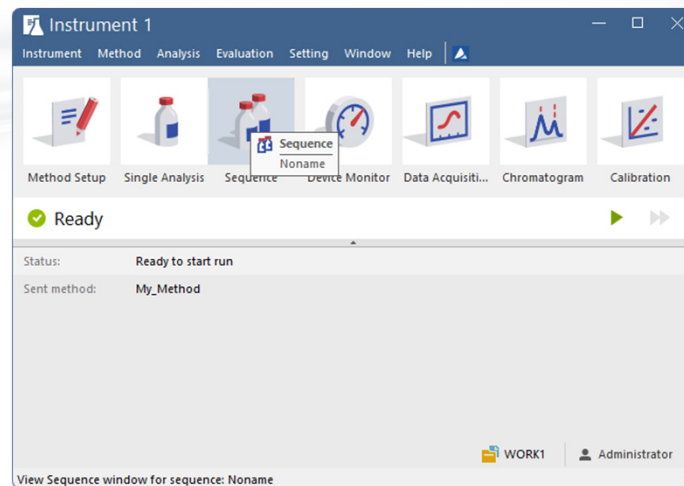
➤ Save as template – saves entire method from chromatogram

- Instrumental part
- Integration
- Linked calibration
- Etc.



SEQUENCE

- Analyze many samples using autosampler
 - Can be used with manual injection
- Utilize optimized method from previous steps



SEQUENCE

SEQUENCE TABLE 1/3

- > Status
- > Vial information
- > Sample information
- > Values for additional calculations
- > Injection volume – important for autosampler

Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Dilution	Inj. Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
	<input checked="" type="checkbox"/>	1	1	1	Std_1	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	1	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	<input checked="" type="checkbox"/>	2	2	1	Std_2	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	2	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	<input checked="" type="checkbox"/>	3	3	1	Std_3	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	3	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	<input checked="" type="checkbox"/>	4	4	1	Std_4	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	4	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	<input checked="" type="checkbox"/>	5	8	2	Sample	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%...	Unknow		Demo 1	Analysis	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	<input type="checkbox"/>															<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

For help press F1. Single Analysis: No method sent - Ready to send method or start sequence Vial: 1 / Inj.: 1

SEQUENCE

SEQUENCE TABLE 2/3

- > File name – usable variables
- > Sample type (+ Levels for standards)
- > Acquisition and printing methods
- > Automated post run actions

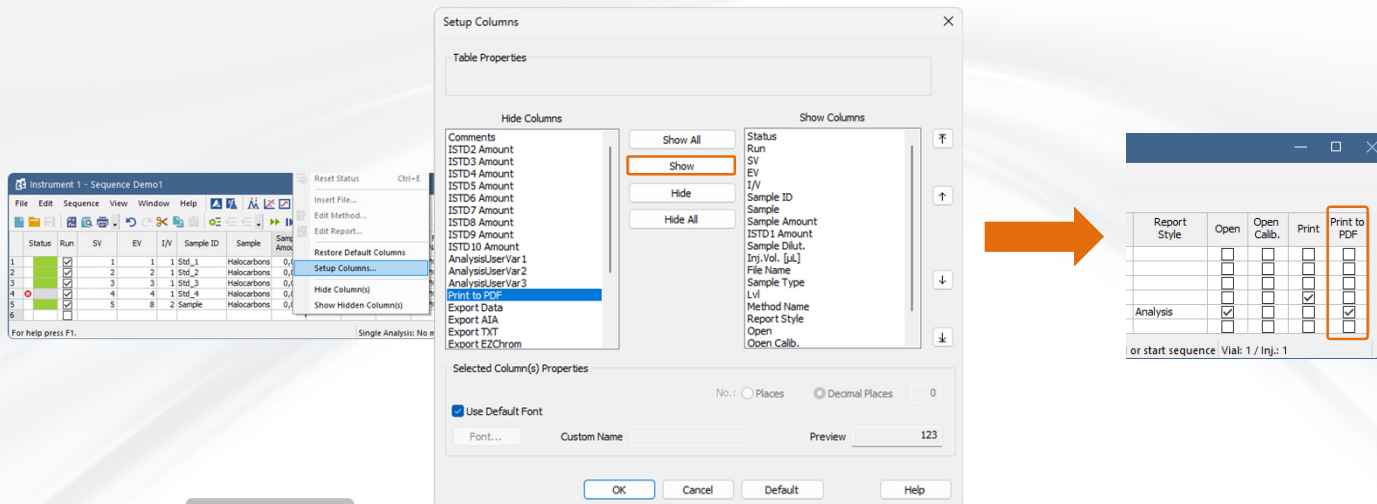
Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Dilution	Inj. Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
	1	1	1	1	Std_1	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	1	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	2	2	2	1	Std_2	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	2	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	3	3	3	1	Std_3	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	3	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	4	4	4	1	Std_4	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%R	Standar	4	Demo 1		<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
	5	8	2		Sample	Halocarbons	0,000	2,000	1,000	5,000	%Q-%q_%...	Unknow		Demo 1	Analysis	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	6															<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

For help press F1. Single Analysis: No method sent - Ready to send method or start sequence | Vial: 1 / Inj.: 1

SEQUENCE

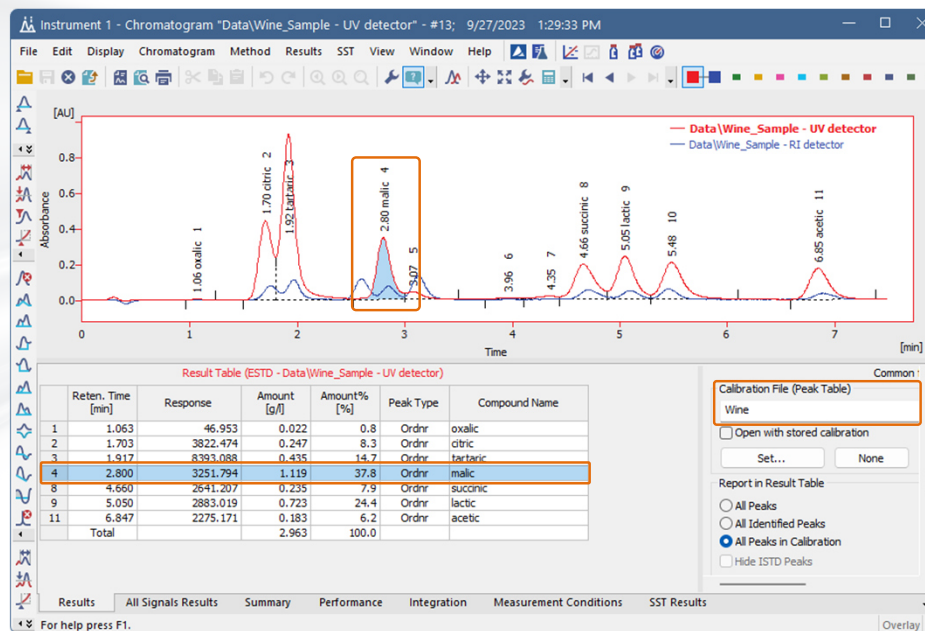
SEQUENCE TABLE 3/3

- ▶ Hidden columns – setup columns dialog
 - Accessible from local menu
 - Applicable to most tables in Clarity



CALIBRATION

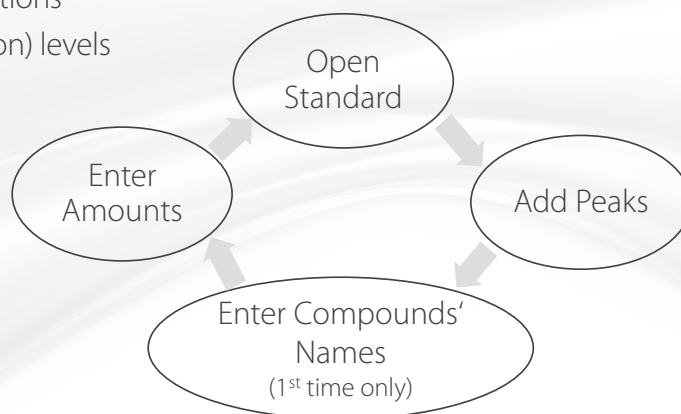
- > Stored as *.cal files
- > Identification of compounds based on retention time



CALIBRATION

MANUAL CREATION

- Acquire and integrate standard samples
- Set calibration options
- Add (concentration) levels



- Save calibration
- Link it to chromatograms

CALIBRATION

CALIBRATION OPTIONS

- > Display mode – ESTD, ISTD etc.
- > Calibration
 - Automatic – recommended
 - Manual – addition of each peak requires manual confirmation
- > Mode
 - Calibrate – peaks added to first empty level
 - Recalibrate – peaks applied to selected level
- > Recalibration
 - Replace – only uses last measured response
 - Average – uses averaged response from “x” measurements
- > Compound units
 - Displayed in result table

Calibration Options (Calib\Wine)

Calibration Options Defaults

Calibration Description: IEX H form, 9 mM H₂SO₄, 0,5 ml/min

Display Mode: ESTD

Number of Signals: 2

Calibration: Automatic Manual

Mode: Calibrate Recalibrate

Curve Check: Deviation 0 % Correlation 0

Apply on: On All Signals On Active Signal

Recalibration: Replace Average

Compound Units: g/l

No. of Points: 10

Recalibration Search Criteria 1 %

Enable Manual Response Value Change

Update Retention Time

Default Injected Volume 0 µL

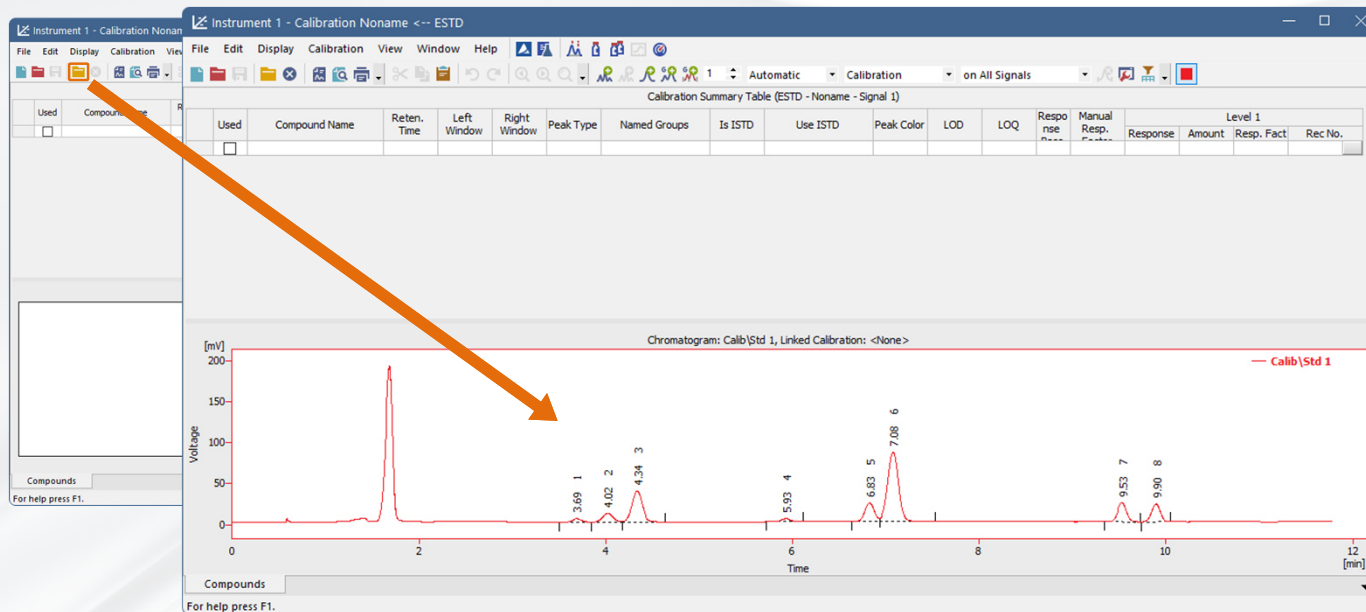
Retention Indexes use Log, Interpolation with Unretained Peak

Response Factor as Response / Amount

OK Cancel Help

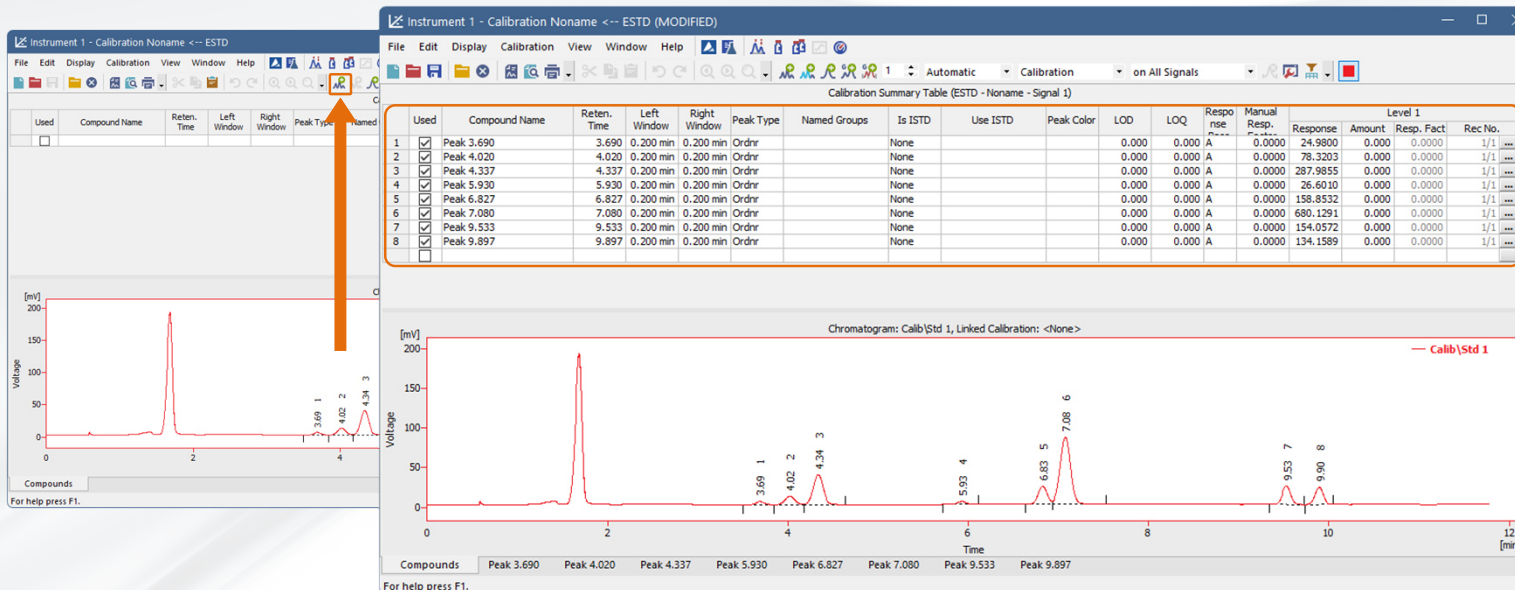
CALIBRATION

FILLING LEVEL 1/4 - OPENING STANDARD



CALIBRATION

FILLING LEVEL 2/4 - ADDING PEAKS



CALIBRATION

FILLING LEVEL 3/4 – NAMING COMPOUNDS (1ST LEVEL ONLY)

Instrument 1 - Calibration Noname <-- ESTD (MODIFIED)

File Edit Display Calibration View Window Help

Automatic Calibration on All Signals

Calibration Summary Table (ESTD - Noname - Signal 1)

Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response	Manual Resp.	Response	Amount	Resp. Fact	Rec No.
<input checked="" type="checkbox"/>	Chloroform	3.690	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	24.9800	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	Trichloroethane	4.020	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	78.3203	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	Tetrachloromethane	4.337	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	287.9855	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	Trichloroethylene	5.930	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	26.6010	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	Bromodichloroethane	6.827	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	158.8532	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	ISTD	7.080	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	680.1291	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	Tetrachloroethylene	9.533	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	154.0572	0.000	0.0000	1/1
<input checked="" type="checkbox"/>	Dibromochloromethane	9.897	0.200 min	0.200 min	Ordnr		None			0.000	0.000	A	0.0000	134.1589	0.000	0.0000	1/1

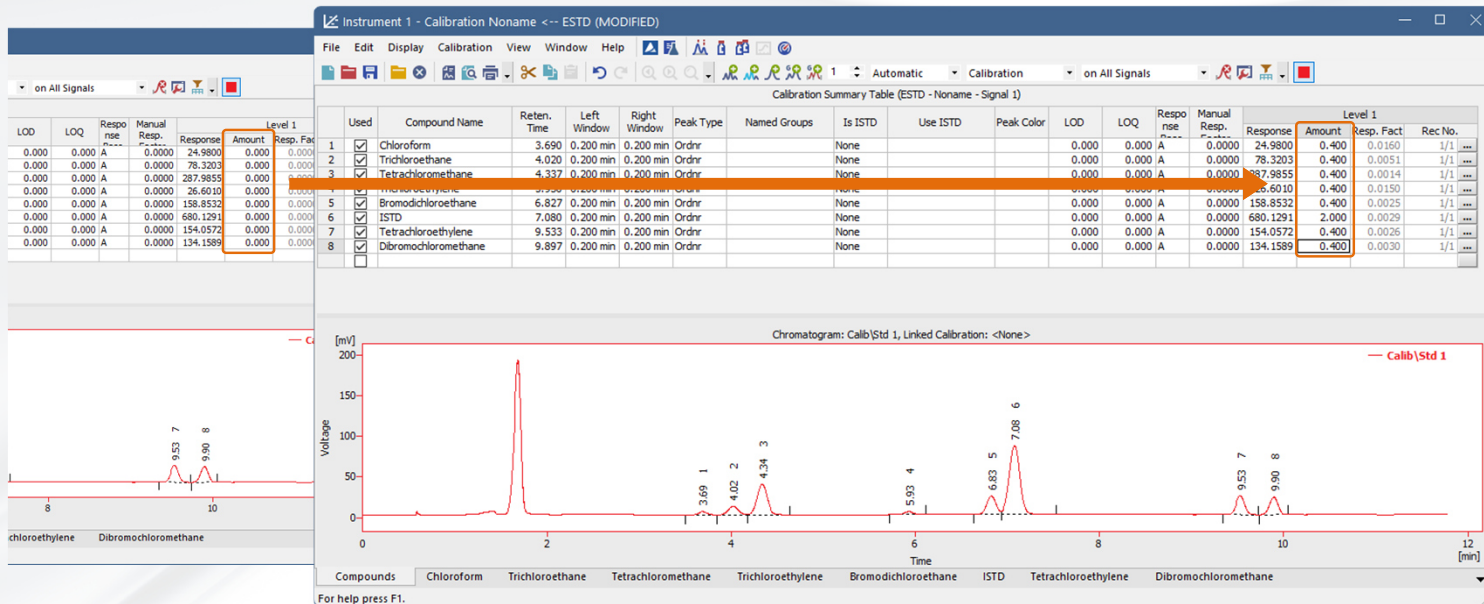
Chromatogram: Calb\Std 1, Linked Calibration: <None>

Compounds: Chloroform Trichloroethane Tetrachloromethane Trichloroethylene Bromodichloroethane ISTD Tetrachloroethylene Dibromochloromethane

For help press F1.

CALIBRATION

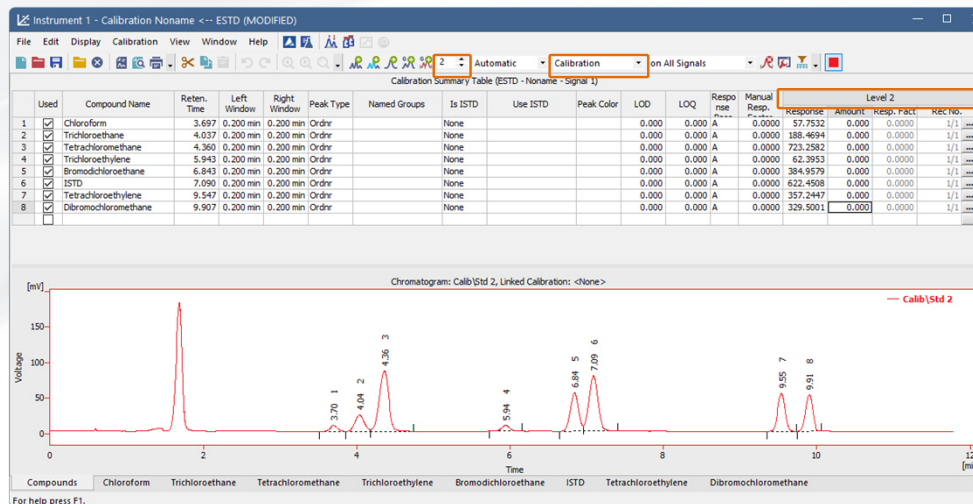
FILLING LEVEL 4/4 – FILLING AMOUNTS



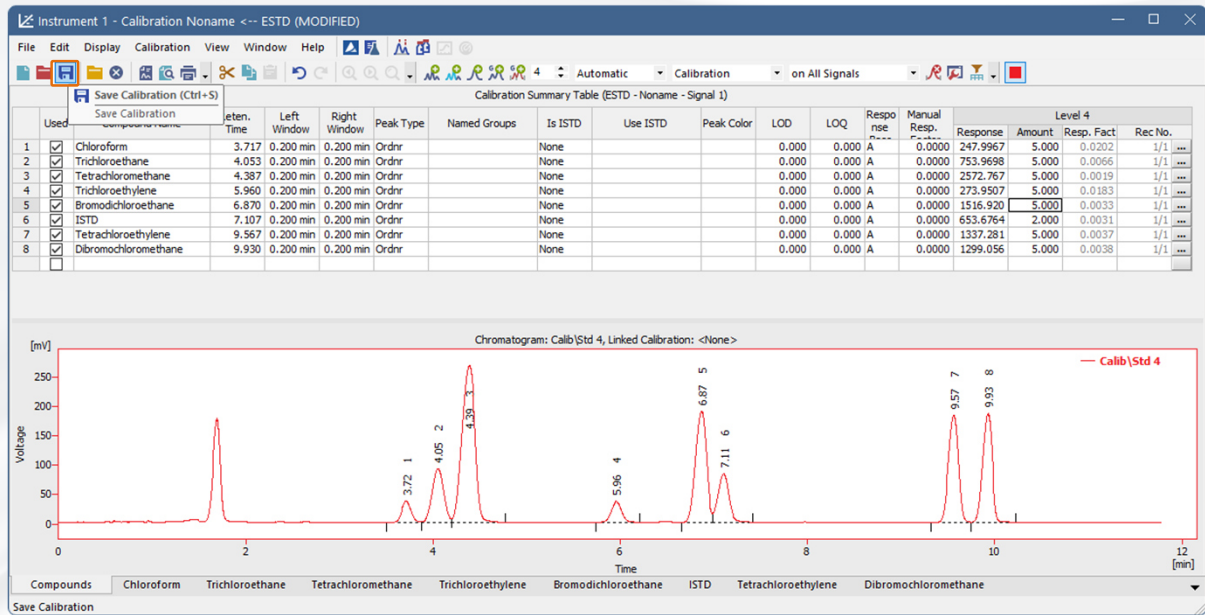
CALIBRATION

NEXT LEVEL

- > Repeat the previous steps for each level
- > Use "Calibration" settings
 - New peaks added to empty level



CALIBRATION SAVING



CALIBRATION

INDIVIDUAL COMPOUND TAB

- Details for the given compound
- Overview of all levels
- How identified
- How quantified
- Calibration curve graph

The screenshot displays the 'Instrument 1 - Calibration' software interface. It features a table of calibration data, a settings panel for identification and quantification, and a calibration curve graph.

Response [mV.s]	Amount [µl]	Resp. Factor	Rec No.	Used
1 28,5632	0,4000	0,0140	1/1	<input checked="" type="checkbox"/>
2 57,2335	1,0000	0,0175	1/1	<input checked="" type="checkbox"/>
3 155,1249	3,0000	0,0193	1/1	<input checked="" type="checkbox"/>
4 247,6095	5,0000	0,0202	1/1	<input checked="" type="checkbox"/>
5 0,0000	0,0000	0,0000	0/0	<input type="checkbox"/>

Identification

Peak Type: Ordnr
Retention Time: 3,717 min
Search Window: Abs
Left Window: 0,2 min
Right Window: 0,2 min
Peak Selection: Nearest

Quantification

Response Base: Area
Is ISTD: None
Use ISTD: ISTD
Curve Fit Type: Linear
Origin: Compute with Origin
Weighting Method: None
Linearization X: None
Linearization Y: None
Correction Factor: 1
Calculate By: []

Calibration Curve

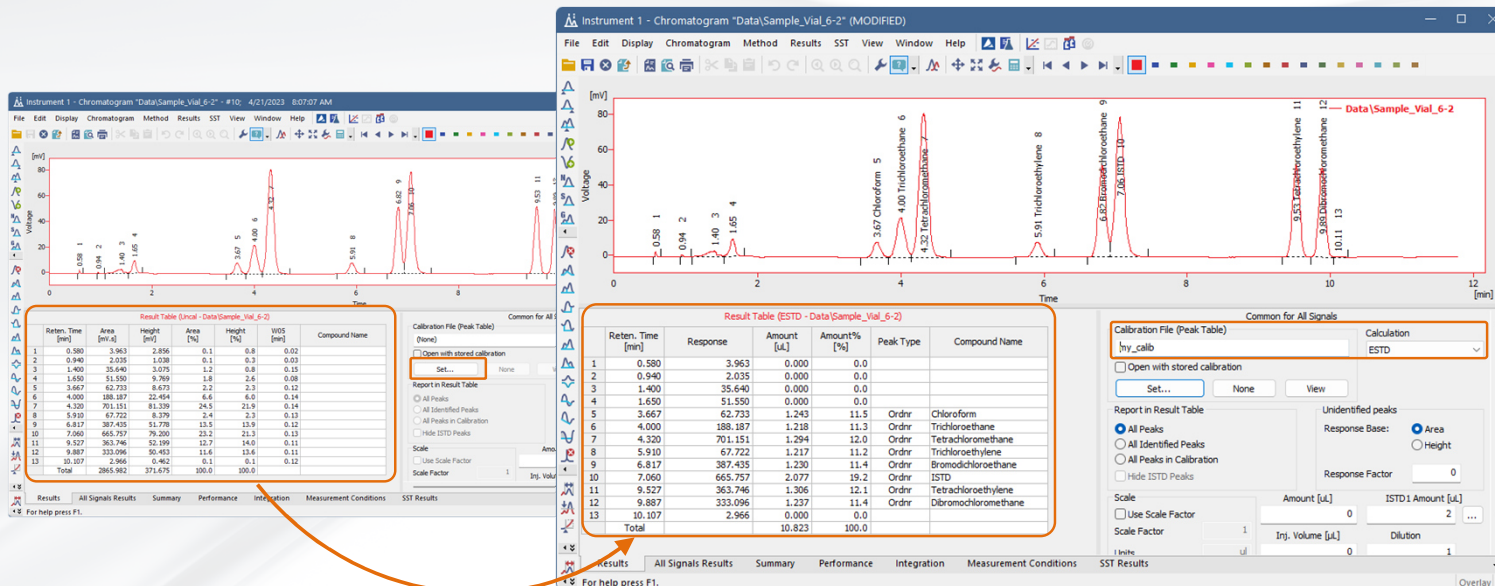
Correlation Coefficient (r): 0,997253
Determination Coefficient (R²): 0,994513
Residium: 0,01046
Equation: $Y = 0,15064 * X + 0,01129$

Graph: Chloroform - 3,717 min, Signal 1. The graph plots Response / ISTD Response (Y-axis, 0.0 to 0.4) against Amount / ISTD Amount (X-axis, 0.0 to 2.5). A linear trendline is shown with four data points marked by '+' symbols.

Compounds: Chloroform, Trichloroethane, Tetrachloromethane, Trichloroethylene, Bromodichloroethane, ISTD, Tetrachloroethylene, Dibromochloromethane

CALIBRATION

LINKING TO CHROMATOGRAM



1 Calibration from method is automatically linked to all measured chromatograms

REPORTS

WHERE TO ENABLE/EXECUTE

- Manually from given window
- Automatically after analysis end
- Batch dialog

The screenshot displays the software interface with three overlapping windows:

- Chromatogram Window:** Shows a chromatogram plot with peaks labeled from 1 to 13. A 'Report Setup' dialog is open over it, with 'Report Setup > Chromatogram' selected.
- Batch Dialog:** A 'Batch' dialog box is open, showing a list of samples and their retention times. The 'Post Run Options' section is highlighted with an orange box, containing:
 - Open in Chromatogram Window
 - Print Results to PDF
 - Export Data
- Single Analysis Dialog:** A 'Single Analysis' dialog box is also visible, with 'Open in Chromatogram Window' checked and highlighted with an orange box.

Instrument 1 - Sequence Demo1

Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dil.	Inj. Vol. [μL]	File Name	Sample Type	Method Name	Report	Open	Open Cal.	Print	Print to PDF
1	1	1	1	1	Halocac...	Std_1	0.400	2.000	1.000	150.000	%Q	Stan	1 Demo1	Calibration	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
2	2	2	2	1	Halocac...	Std_2	1.000	2.000	1.000	150.000	%Q	Stan	2 Demo1	Calibration	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3	3	3	3	1	Halocac...	Std_3	3.000	2.000	1.000	150.000	%Q	Stan	3 Demo1	Calibration	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
4	4	1	1	1	Halocac...	Std_4	5.000	2.000	1.000	150.000	%Q	Stan	4 Demo1	Calibration	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
5	5	8	2	1	Halocac...	Sample	5.000	2.000	1.000	150.000	%Q	Unkn	Demo1	Analysis	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
6																		

REPORTS

REPORT SETUP

- "Printing method" set separately for each window
- *.sty files in COMMON folder

The screenshot displays two windows from the DataApex software. The left window, titled 'Instrument 1 - Chromatogram "DataSample_Vial_6-2" - #10: 4/21/2023 8:07:07 AM', shows the 'Report Setup Chromatogram' dialog. The 'Print' checkbox is checked, and the 'Report Style' is set to 'Analysis'. The right window, titled 'Instrument 1 - Sequence Demo', shows a data table with columns for Status, Run, SV, EV, I/V, Sample ID, Sample, Sample Amount, ISTD1 Amount, Sample Dilut., Inj. Vol. [µL], File Name, Sample Type, Lvl, Method Name, Report Style, Open, Open Calib., and Print. The 'Report Style' column is set to 'Analysis'. Below the table, the 'Report Setup Analysis' dialog is open, showing options for 'Open in Chromatogram Window', 'Print Results', 'Print Results To PDF', and 'Export Data'. The 'Report Style' dropdown is set to 'Analysis', and the 'Print Background Color of Graphs' checkbox is checked.

Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj. Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
	1		1	1	Halocar...	Std_1	0.400	2.000	1.000	150.000	%Q	Stan	1	Demo1	Analysis	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

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