



USER TRAINING

ADVANCED – PART 2

P008/80C 04/2022



Agenda

- Calibration
 - Details of calibration point
 - Calibration options
 - LOD, LOQ
 - Bracketing and Standard Addition
- Calculations
 - ISTD and Normalized %
- Groups
- Scale and uncalibrated response
- Dilution
- Injection volume
 - Single analysis and calibration options
 - Autosampler in single run
- User variables



CALIBRATION → DETAILS OF CALIBRATION POINT

The screenshot shows the 'Instrument 1 - Calibration Calib\Demo1 <-- ISTD (MODIFIED)' window. It features a menu bar (File, Edit, Display, Calibration, View, Window, Help), a toolbar, and a main workspace. The workspace is divided into a table of calibration points on the left and a graph on the right. The graph is titled 'Tetrachloroethylene - 9,547 min, Signal 1' and shows a linear relationship between 'Amount / ISTD1 Amount' (x-axis, 0.0 to 2.5) and 'Response' (y-axis, 0.0 to 2.0). A data point is marked with a '+' and a vertical error bar. A callout bubble points to the 'Used' checkbox in the table for the first level, which is checked. Another callout bubble points to the 'Details of Calibration Point' dialog box, which displays a table of data for the selected level.

Response [mV.s]	Amount [u]	Resp. Factor	Rec No.	Used
1 255,4962	0,4000	0,0016	2/2	<input checked="" type="checkbox"/>
2 357,1732	1,0000	0,0028	1/1	<input checked="" type="checkbox"/>
3 894,8096	3,0000	0,0034	1/1	<input checked="" type="checkbox"/>
4 1335,148	5,0000	0,0037	1/1	<input checked="" type="checkbox"/>
5 0,0000	0,0000	0,0000	0/0	<input type="checkbox"/>

Used Level	Used	Ret. time	Amount	Area	Height	Date	Standard
1	<input checked="" type="checkbox"/>	9,5333		153,8191	23,6682	12.05.2020 14:35:14	"C:\Clarity83\DataFiles\DEMO1\Calib\Std 1.prm"
2	<input checked="" type="checkbox"/>	9,5467	0,4000	357,1732	53,0401	12.05.2020 14:35:28	"C:\Clarity83\DataFiles\DEMO1\Calib\Std 2.prm"

Calibration Curve
Correlation Factor: 0,9904507
Residuum: 0,14521
Equation: $Y = 0,86895 * X$

(Un)check checkbox to include/omitt from calibration

Residual sum of deviation squares

Menu Calibration / Show Details displays data used for selected level



Calibration Options (Calib\Demo1) ? X

Calibration Options Defaults

Calibration Description:

Display Mode: ISTD

Number of Signals: 1

Calibration: Automatic Manual

Mode: Calibrate Recalibrate

Curve Check: Deviation 5 %

Correlation 0,995

Apply on: On All Signals On Active Signal

Recalibration: Replace Average

Compound Units: ul

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

Refers to **automatic** or **manual** calibration

Calculation types: ESTD, ISTD, NORM, STDADD

Calibration curve check: **Failure** displayed in the **Peak Type** column in **Result Table**



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 Retention Time Peak From Standard: 3,697 min Compound Current: 3,697 min Update: On	Amount: 1 ul Response Base: Area Response [mV.s]: Current: 57,01 → From Standard: 57,23 → Resulting: 57,12 Departure: 0,22 mV.s (0,38 %)

<< Less Next Skip C Help

Refers to the **level** being **calibrated**

Criteria for identification

Information about the compound

Response options: Area, Height or Area %

Resulting response

Adjust response manually

Original response

Suggested response from standard



CALIBRATION → LOD, LOQ

Instrument 1 - Calibration Calib\ASTM6730_C5-C15-RI <-- ESTD

File Edit Display Calibration View Window Help

Calibration Summary Table (ESTD - Calib\ASTM6730_C5-C15-RI - Signal 1)

Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Is ISTD	Use ISTD	Reten. Index	LOD	LOQ	Response Base	Manual Resp. Factor	Level 1				
													Response	Amount	Resp. Fact	Rec No.	
1	✓	n-Pentane	12,857	0,200 min	0,200 min	Ordnr	None		500,000	0,100	0,300	A	0,0000	4724,4275	0,000	0,0000	1/1 ...
2	✓	n-Hexane	20,500	0,200 min	0,200 min	Ordnr	None		600,000	0,100	0,300	A	0,0000	4384,6177	0,000	0,0000	1/1 ...
3	✓	n-Heptane	28,880	0,200 min	0,200 min	Ordnr	None		700,000	0,100	0,300	A	0,0000				1/1 ...
4	✓	n-Octane	38,693	0,200 min	0,200 min	Ordnr	None		800,000	0,100	0,300	A	0,0000	10596,7032	0,000	0,0000	1/1 ...
5	✓	n-Nonane	49,687	0,200 min	0,200 min	Ordnr	None		900,000	0,100	0,300	A	0,0000	11577,5428	0,000	0,0000	1/1 ...
6	✓	n-Decane	61,063	0,200 min	0,200 min	Ordnr	None		1000,000	0,100	0,300	A	0,0000	6271,1765	0,000	0,0000	1/1 ...
7	✓	n-Undecane	72,393	0,200 min	0,200 min	Ordnr	None		1100,000	0,100	0,300	A	0,0000	12734,3308	0,000	0,0000	1/1 ...
8	✓	n-Dodecane	83,017	0,200 min	0,200 min	Ordnr	None		1200,000	0,100	0,300	A	0,0000	6416,3005	0,000	0,0000	1/1 ...
9	✓	n-Tridecane	93,273	0,200 min	0,200 min	Ordnr	None		1300,000	0,100	0,300	A	0,0000	13119,1941	0,000	0,0000	1/1 ...
10	✓	n-Tetradecane	102,720	0,200 min	0,200 min	Ordnr	None		1400,000	0,100	0,300	A	0,0000	6801,6947	0,000	0,0000	1/1 ...
11	✓	n-Pentadecane	111,883	0,200 min	0,200 min	Ordnr	None										1/1 ...

Column for Retention (Kovats) indexes is hidden in default settings. Use setup columns to display it.

Amounts lower than specified LOD or LOQ limits are marked in Peak type column.

Instrument 1 - Chromatogram "Data\N_PARAFFINS_FOR_ASTM6730 - Detector A" - #8; 04.02.2020 15:25:08

File Edit Display Chromatogram Method Results SST DHA 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	2294,657	0,000	< LOD Ordnr Free	n-Pentane
2	20,430	3455,578	0,000	< LOD Ordnr Free	n-Hexane
3	28,863	6441,917	0,000	< LOD Ordnr Free	n-Heptane
4	38,673	7031,387	0,000	< LOD Ordnr Free	n-Octane
5	49,657	7115,519	0,000	< LOD Ordnr Free	n-Nonane
6	61,087	7554,321	0,000	< LOD Ordnr Free	n-Decane
7	72,323	7411,802	0,000	< LOD Ordnr Free	n-Undecane
		6253,795	0,000	< LOD Ordnr Free	n-Dodecane
		8063,347	0,000	< LOD Ordnr Free	n-Tridecane
10	102,747	8063,347	0,000	< LOD Ordnr Free	n-Tetradecane
11	111,750	7502,488	0,000	< LOD Ordnr Free	n-Pentadecane
Total			0,000		

Common for All Signals

Calibration File (Peak Table): ASTM6730_C5-C15-RI

Calculation: ESTD

Integration Algorithm: 8.0

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
- Amount [mg]: 0
- ISTD 1 Amount [mg]: 0
- Inj. Volume [µL]:
- Dilution:



CALIBRATION → BRACKETING & STANDARD ADDITION

This calibration will be used once „**Calibration used as specified by user**“ option is selected

Method Setup Demo1 (MODIFIED)

Common for all detectors

Calibration File (Peak Table): Example

Calculations: ESTD, Integration Algorithm: 8.0

Unidentified Peaks: Response Base: Area, Response Factor: 0 [Am/Rsp]

Calibration Cloning In Sequence: %s %R

Report in Result Table: All Peaks in Calibration

Send Method

Copy of the Example calibration will be created according to Sequence options, Calibration and Sequence Usage

Sequence Options

Description:

Sequence mode: Active, Idle time: 0 [min]

Run lines: 1-5

Counter (%n): 1

Solve conflict of filename: Automatically

Calibration and sequence usage: Calibration used as specified by user

After sequence is finished: Send shutdown method, Run shutdown method, Sample type: Bypass, Vial no.: 1, Inj. vol. [µL]: 0

OK

Calibration and Sequence Usage:
Clone calibration at each Sequence start
Standard Addition
Bracketing



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Instrument 1 - Calibration Calib\Demo1 <-- ISTD

Response [mV.s]	Amount [ul]	Resp. Factor	Rec No.	Used	
1	678,5633	2,0000	0,0029	1/1	✓
2	624,1404	2,0000	0,0032	1/1	✓
3	611,2742	2,0000	0,0033	1/1	✓
4	656,9457	2,0000	0,0030	1/1	✓
5	0,0000	0,0000	0,0000	0/0	✗
6	0,0000	0,0000	0,0000	0/0	✗
7	0,0000	0,0000	0,0000	0/0	✗
8	0,0000	0,0000	0,0000	0/0	✗
9	0,0000	0,0000	0,0000	0/0	✗
10	0,0000	0,0000	0,0000	0/0	✗
11	0,0000	0,0000	0,0000	0/0	✗

ISTD amount of compound in standard

Left Window: [] min
Right Window: 0,2 min

Peak Selection: Nearest

Quantification: Response Base: Area, Is ISTD: ISTD1, Use ISTD: [], Curve Fit Type: Linear, Origin: Curve passes through Origin, Weighting Method: None, Linearization X: None, Linearization Y: None, Correction Factor: 1, Calculate By: []

Compounds: Chloroform, Trichloroethane, Tetrachlormethane, Trichloroethene

For Help, press F1

Up to 10 ISTD compounds allowed in calibration. If conditions are not met, no results will be calculated

Instrument 1 - Chromatogram "Data\Sample_Vial_9-2" (MODIFIED)

ISTD - 7,107 min, Signal 1

Chromatogram showing peaks at retention times: 3,66 Chloroform 5, 3,99 Trichloroethane 6, 4,32 Tetrachlormethane 7, 5,90 Trichloroethene 8, 6,42 9, 6,80 Bromodichloroethane 10, 7,05 ISTD 11, 7,92 12, 9,13 13, 9,14 14.

Result Table (ISTD - Data\Sample_Vial_9-2)

Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
5	3,660	148,283	2,806	14,3	Ordnr (by ISTD1) Chloroform
6	3,990	442,673	2,731	13,9	Ordnr (by ISTD1) Trichloroethane
7	4,320	1611,800	2,831	14,4	Ordnr (by ISTD1) Tetrachlormethane
8	5,897	164,768	2,823	14,4	Ordnr (by ISTD1) Trichloroethene
10	6,800	913,399	2,765	14,1	Ordnr (by ISTD1) Bromodichloroethane
11	7,047	674,644	ISTD	ISTD	ISTD
13	9,510	827,904	2,836	14,4	Ordnr (by ISTD1) Tetrachloroethyle
14	9,870	800,385	2,845	14,5	Ordnr (by ISTD1) Dibromochloromet
Total			19,636	100,0	

Common for All Signals

Calculation: ISTD

Integration Algorithm: 8.0

Report in Result Table: All Peaks

Unidentified peaks: Base: Area

ISTD compound amount in sample

Scale: Amount [ul]: 0, ISTD1 Amount [ul]: 2

Scale Factor: 1, Inj. Volume [ul]: 0, Dilution: 1

User Variables: []

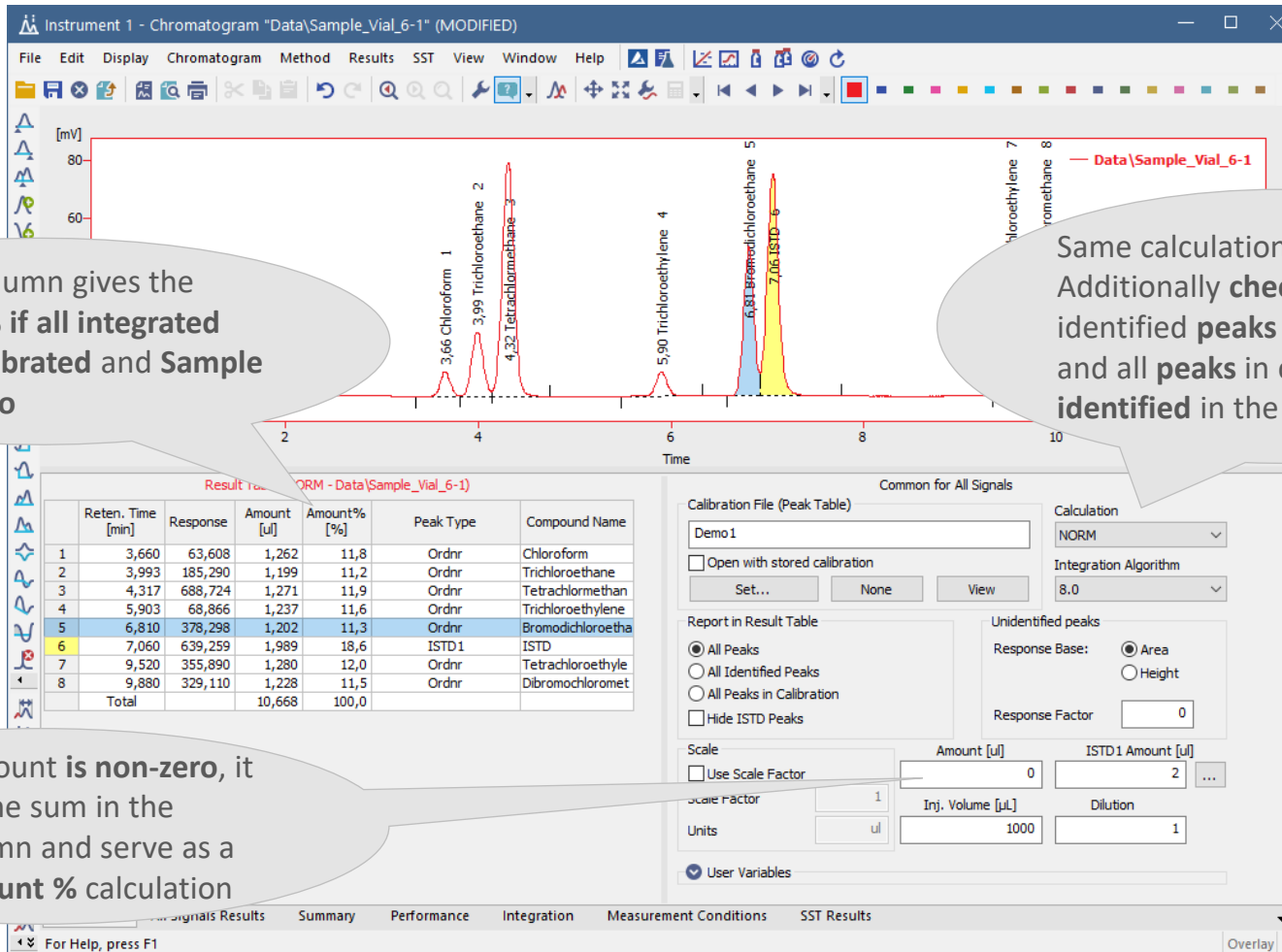
Results | All Signals Results | Summary | Performance | Integration | Measurement Conditions | SST Results

For Help, press F1

ISTD calculations are performed:
a) Amount for ISTD is set in both calibration and sample
b) both are zero



CALCULATIONS → NORMALIZED %



Amount % column gives the normalized % if all integrated peaks are calibrated and Sample amount is zero

Same calculations to ESTD Additionally checks that that all identified peaks are calibrated and all peaks in calibration were identified in the chromatogram

If Sample amount is non-zero, it will replace the sum in the Amount column and serve as a base for Amount % calculation



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→ User variables



GROUPS → ADDING A GROUP

1st step is to name them and add peaks to a group in the integration table

2nd step is to set a Group in Calibration table. The compound name and amount is set as for ordinary peaks

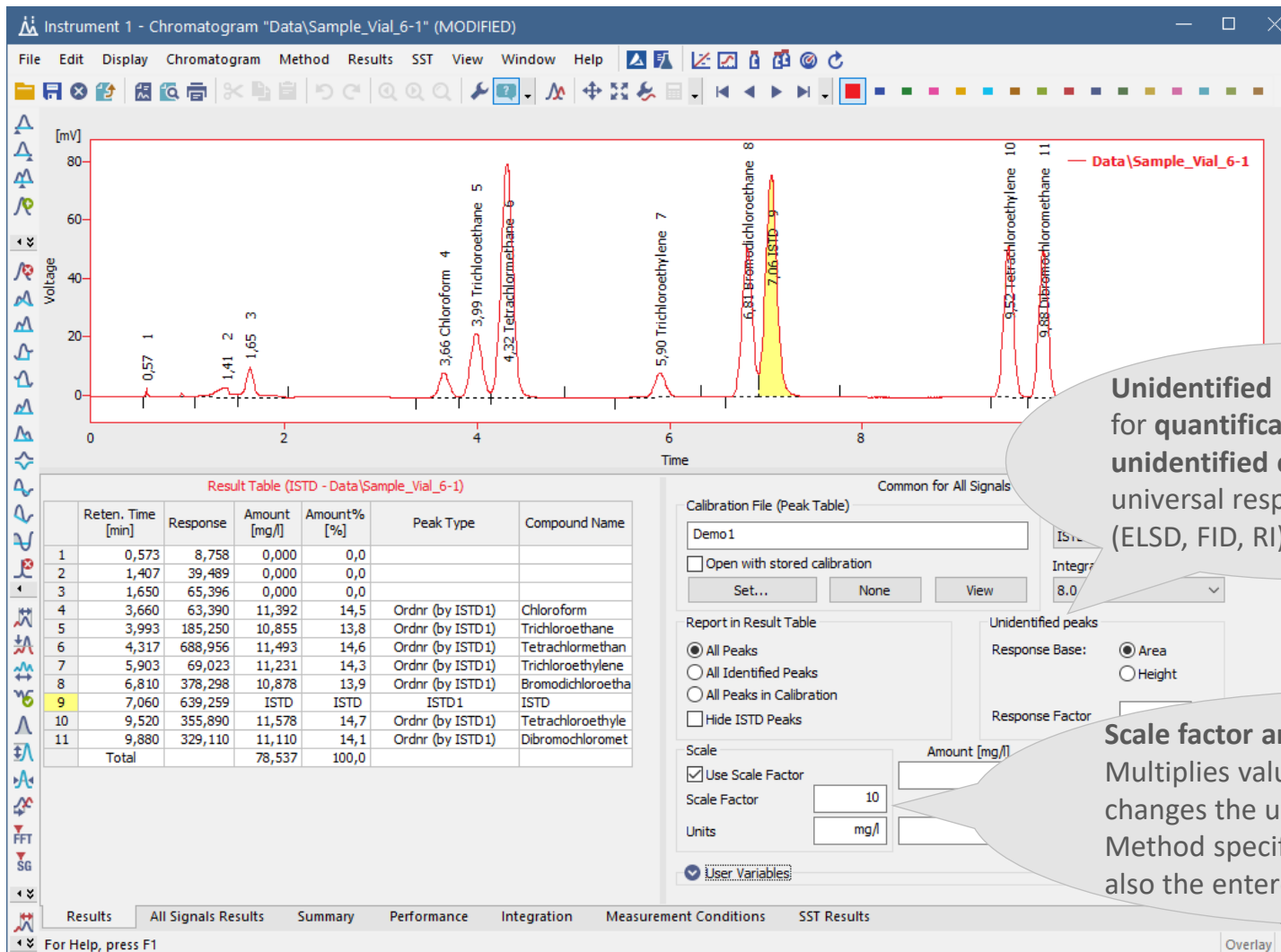
Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	ISTD	Use ISTD	Peak Color	Response Base	Manual Resp. Factor	Response	Amount	Resp. Fact	Rec No.
<input checked="" type="checkbox"/>	Chloroform	3,717	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Trichloroethane	4,053	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Tetrachloromethane	4,387	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Trichloroethylene	5,960	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Bromodichloroethane	6,870	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	ISTD	7,107	0,200 min	0,200 min	Ordnr		ISTD1		A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Tetrachloroethylene	9,567	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Dibromochloromethane	9,930	0,200 min	0,200 min	Ordnr		None	ISTD	A	0,0000	0,0000	0,0000	0,000	0,0000	0/0
<input checked="" type="checkbox"/>	Group B				Grp_B		None	ISTD	A	0,0000	1017,556	0,000	0,000	0,0000	1/1
<input checked="" type="checkbox"/>	Group A				Grp_A		None	ISTD	A	0,0000	684,9996	0,000	0,000	0,0000	1/1

Chromatogram: Sample_Vial_6-1, Linked Calibration: Demo 1

Compounds: Chloroform Trichloroethane Tetrachloromethane Trichloroethylene Bromodichloroethane ISTD Tetrachloroethylene Group A



CHROMATOGRAM WINDOW → SCALE & UNCAL RESPONSE

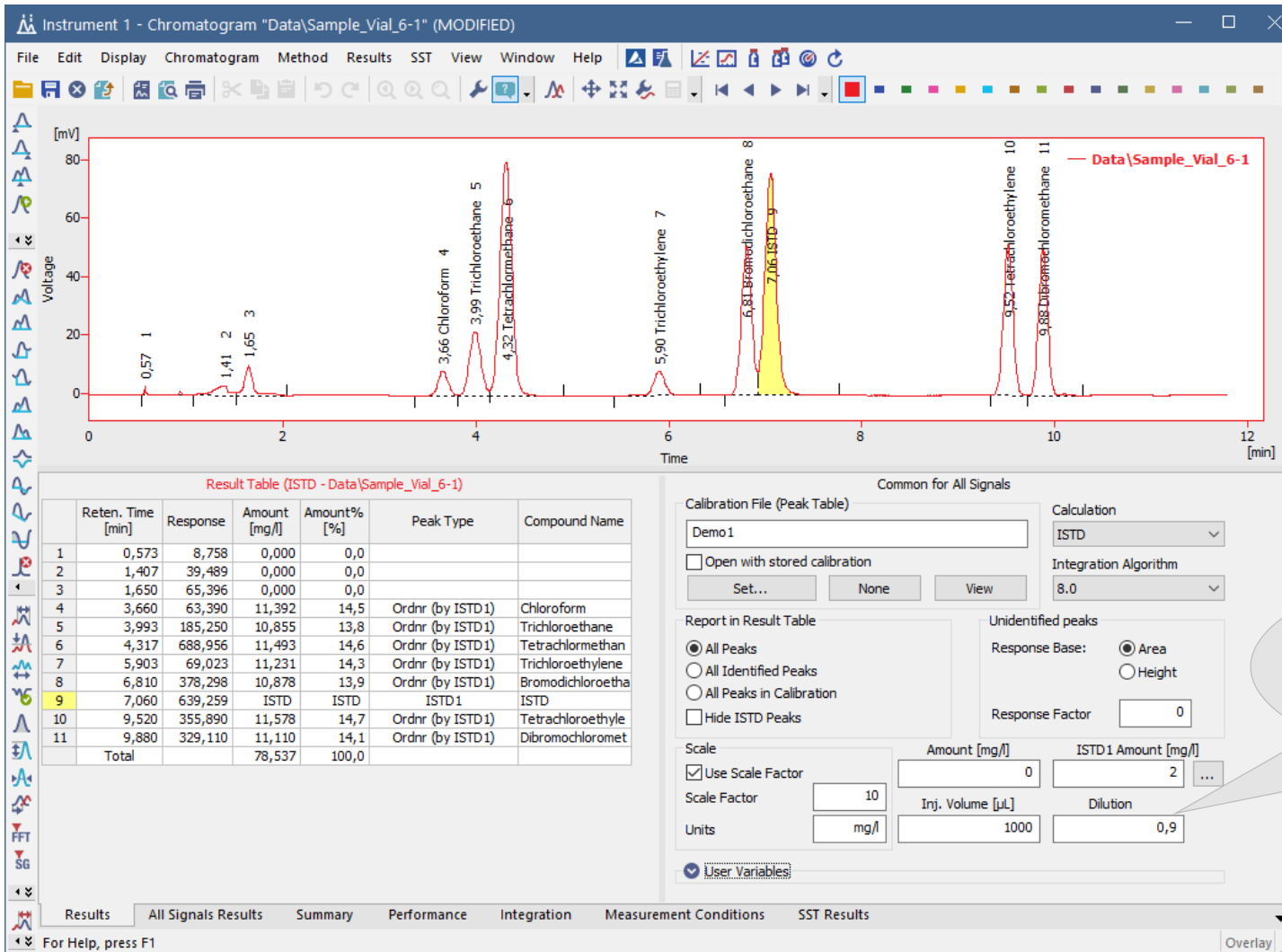


Unidentified peaks are used for quantification of unidentified compounds. For universal response detectors (ELSD, FID, RI)

Scale factor and Units upon scaling: Multiplies values in Amount column and changes the units in column header. Method specific parameter, multiplies also the entered Sample Amount value.



CHROMATOGRAM WINDOW → SCALE & UNCAL RESPONSE



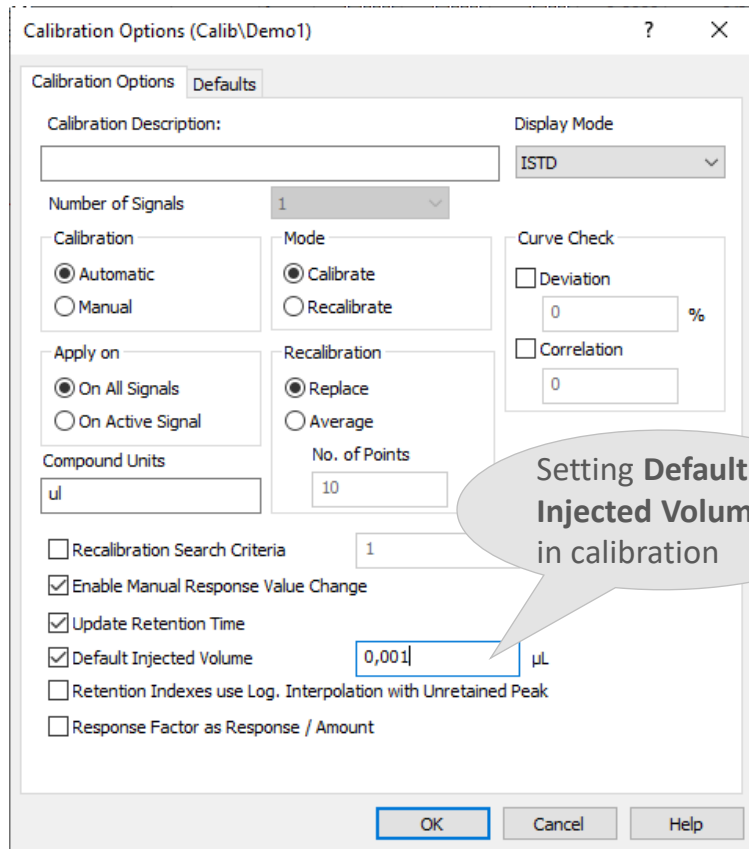
Dilution:
 Multiplies values in Amount column.
 Sample specific parameter (entered from Sequence or Single Analysis window).



INJECTION VOLUME → SINGLE ANALYSIS & CALIBRATION OPTIONS

Default Injection Volume must be set first in calibration and Injection Volume set in standards before calibrating

Supposes **linear detector** response
Improper use may lead to **incorrect results**



Calibration Options (Calib\Demo1)

Calibration Options Defaults

Calibration Description: Display Mode: ISTD

Number of Signals: 1

Calibration: Automatic Manual

Mode: Calibrate Recalibrate

Curve Check: Deviation Correlation

Apply on: On All Signals On Active Signal

Recalibration: Replace Average

Compound Units: ul No. of Points: 10

Recalibration Search Criteria: 1

Enable Manual Response Value Change

Update Retention Time

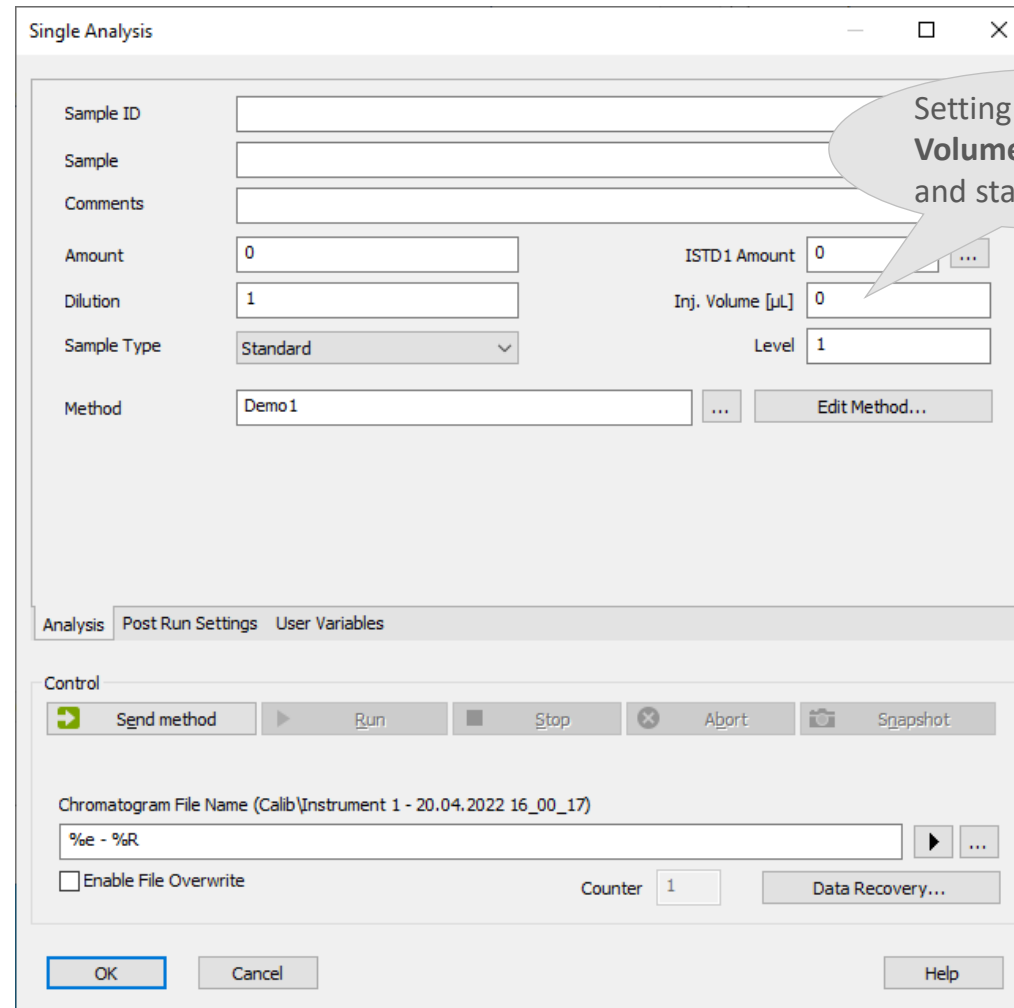
Default Injected Volume: 0,001 μL

Retention Indexes use Log. Interpolation with Unretained Peak

Response Factor as Response / Amount

OK Cancel Help

Setting Default Injected Volume in calibration



Single Analysis

Sample ID:

Sample:

Comments:

Amount: 0 ISTD1 Amount: 0

Dilution: 1 Inj. Volume [μL]: 0

Sample Type: Standard Level: 1

Method: Demo1 Edit Method...

Analysis Post Run Settings User Variables

Control: Send method Run Stop Abort Snapshot

Chromatogram File Name (Calib\Instrument 1 - 20.04.2022 16_00_17): %e - %R

Enable File Overwrite Counter: 1 Data Recovery...

OK Cancel Help

Setting Injection Volume for sample and standard



SINGLE ANALYSIS → USE AUTOSAMPLER

Single Analysis

Sample ID

Sample

Comments

Amount 0 ISTD1 Amount 0

Dilution 1 Inj. Volume [µL] 15

Sample Type Standard Level 1

Method Default1 Edit Method...

Analysis Post Run Settings User Variables

Control

Send method Inject & Run Stop Abort Snapshot

Use Autosampler Vial 1

Chromatogram File Name (Calib\Instrument 1 - 20.04.2022 16_05_25)

%e - %R

Enable File Overwrite Counter 1 Data Recovery...

OK Cancel Help

Perform one injection from the **specified Vial** and start the acquisition

Use Autosampler – option **enabled** only if AS is configured on the instrument

Support for **graphical entry** of vial number



SINGLE ANALYSIS → USER VARIABLES

Instrument 1 - Chromatogram "Data\Sample_Vial_6-1" (MODIFIED)

Result Table (ISTD - Data\Sample_Vial_6-1)

Reten. Time [min]	Response	Amount [µl]	Amount% [%]	Peak Type	Compound Name
0,57					
1,41					
1,65					
3,66	63,390	1,266	14,5	Ordnr (by ISTD1)	Chloroform
3,99	185,250	1,206	13,8	Ordnr (by ISTD1)	Trichloroethane
4,31	688,956	1,277	14,6	Ordnr (by ISTD1)	Tetrachlormethan
4,32					
5,90	69,023	1,248	14,3	Ordnr (by ISTD1)	Trichloroethylene
6,81	378,298	1,209	13,9	Ordnr (by ISTD1)	Bromodichloroetha
7,06	639,259	ISTD	ISTD	ISTD1	
7,06					
9,52	355,890	1,286	14,7	Ordnr (by ISTD1)	Tetrachloroethyle
9,880	329,110	1,234	14,1	Ordnr (by ISTD1)	Dibromochloromet
Total		8,726	100,0		

User Variables

Name	Value
1 my variable 1	10
2 my variable 2	20
3 my variable 3	-20

Analysis variables can be used further in the custom calculations in the Result table

Single Analysis

Name	Value	
Variable 1	my variable 1	10
Variable 2	my variable 2	20
Variable 3	my variable 3	-20

Control

Send method Inject & Run Stop Abort Snapshot

Use Autosampler Vial 1:A1

Chromatogram File Name (Calib\Instrument 1 - 14.05.2020 12_51_10)

%e - %R

Enable File Overwrite Counter 1 Data Recovery...

OK Cancel Help

Analysis user variables are copied from the single analysis to the measured chromatogram



SEQUENCE → USER VARIABLES

The screenshot displays the 'Instrument 1 - Sequence Demo1' window. It features a chromatogram on the left, a sequence table in the center, a result table at the bottom left, and a configuration window at the bottom right. An orange arrow points from the 'my variable 3' column in the sequence table to the 'my variable 3' row in the 'User Variables' configuration window. A speech bubble on the right says 'Add user variables columns using Setup columns.' and another on the bottom left says 'Analysis variables can be used further in the custom calculations in the Result table'.

Sequence Table:

Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [μL]	my variable 1	my variable 2	my variable 3	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.
1	1:A1	1:A1	1	Halocar...	Std_1	0,400	2,000	1,000	5,000	10,000	20,000	-20,000	%Q	Stan	1	Demo 1	Calibration			
2	1:B1	1:B1	1	Halocar...	Std_2	1,000	2,000	1,000	5,000	10,000	20,000	-20,000	%Q	Stan	2	Demo 1	Calibration			
3	1:C1	1:C1	1	Halocar...	Std_3	3,000	2,000	1,000	5,000	10,000	20,000	-20,000	%Q	Stan	3	Demo 1	Calibration			
4	1:D1	1:D1	1	Halocar...	Std_4	5,000	2,000	1,000	5,000	10,000	20,000	-20,000	%Q	Stan	4	Demo 1	Calibration			
5	1:E1	1:B2	2	Halocar...	Sample	5,000	2,000	1,000	5,000	10,000	20,000	-20,000	%Q Vial_...	Unkn		Demo 1	Analysis			

Result Table (ISTD - Data\Sample_Vial_6-1):

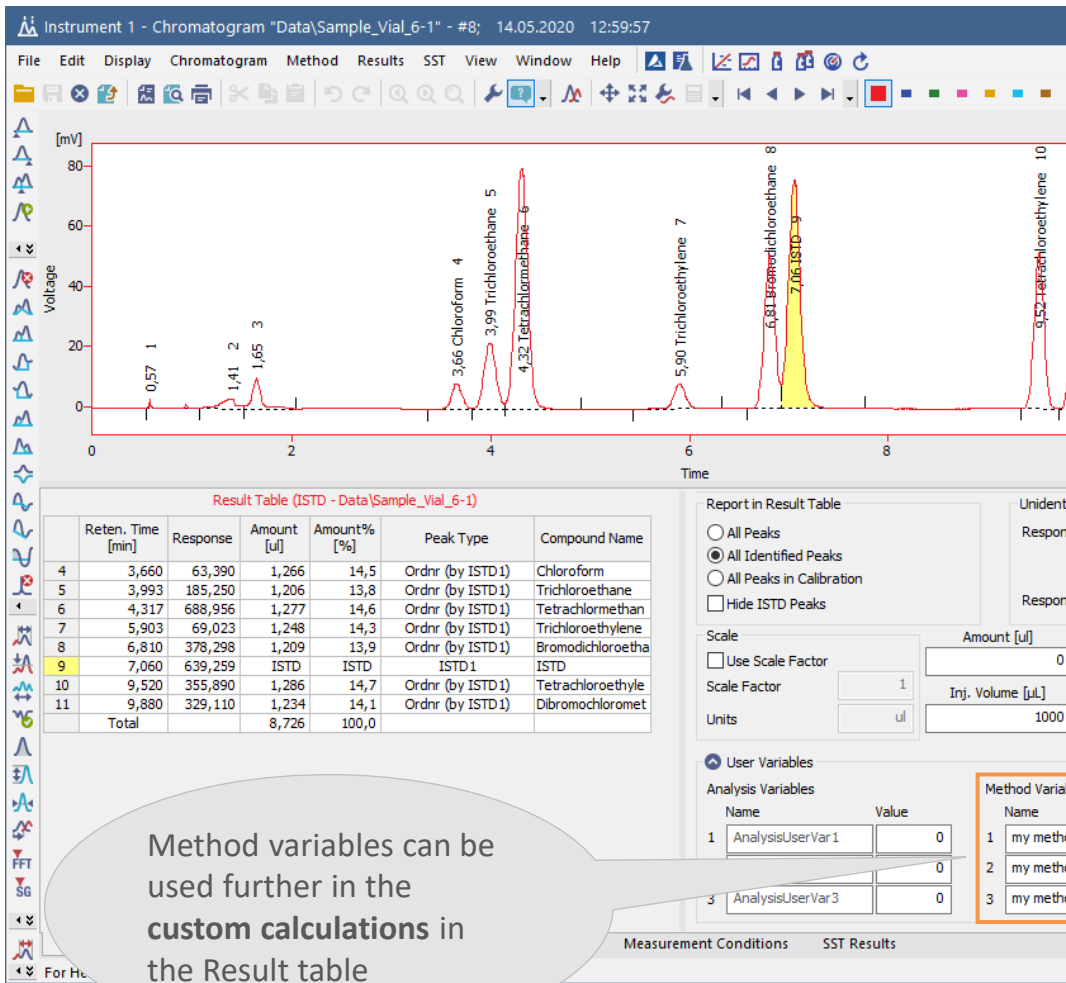
Reten. Time [min]	Response	Amount [μl]	Amount% [%]	Peak Type	Compound Name
4	3,660	63,390	1,266	14,5	Chloroform
5	3,993	185,250	1,206	13,8	Trichloroethane
6	4,317	688,956	1,277	14,6	Tetrachlormethan
7	5,903	69,023	1,248	14,3	Trichloroethylene
8	6,810	378,298	1,209	13,9	Bromodichloroetha
9	7,060	639,259	ISTD	ISTD	ISTD
10	9,520	355,890	1,286	14,7	Tetrachloroethyle
11	9,880	329,110	1,234	14,1	Dibromochloromet
Total			8,726	100,0	

User Variables Configuration:

Analysis Variables		Method Variables	
Name	Value	Name	Value
1 my variable 1	10	1 MethodUserVar1	0
2 my variable 2	20	2 MethodUserVar2	0
3 my variable 3	-20	3 MethodUserVar3	0



METHOD SETUP → METHOD VARIABLES



Method Setup Demo1 (MODIFIED)

Common for all detectors

Subtraction
Chromatogram: [None]
Matching: No Change

Column Calculations
Unretained Time: 0 [min]
Column Length: 25000 [mm]
 Statistical Moments
 From Width at 50%

User Variables

Variable	Name	Value
Variable 1	my method variable 1	40
Variable 2	my method variable 2	50
Variable 3	my method variable 3	-60

Event Table AS Measurement Acquisition Integration Calculation Advanced

OK Cancel Send Method

Method variables can be used further in the custom calculations in the Result table

Advanced tab of the method - user variables are copied from the Method Setup to the measured chromatogram



...THANK YOU FOR YOUR TIME



SUPPORT@DATAAPEX.COM
WWW.DATAAPEX.COM