DataApex

SMART SOLUTION FOR LABORATORIES

Clarity™

advanced chromatography software

USER TRAINING

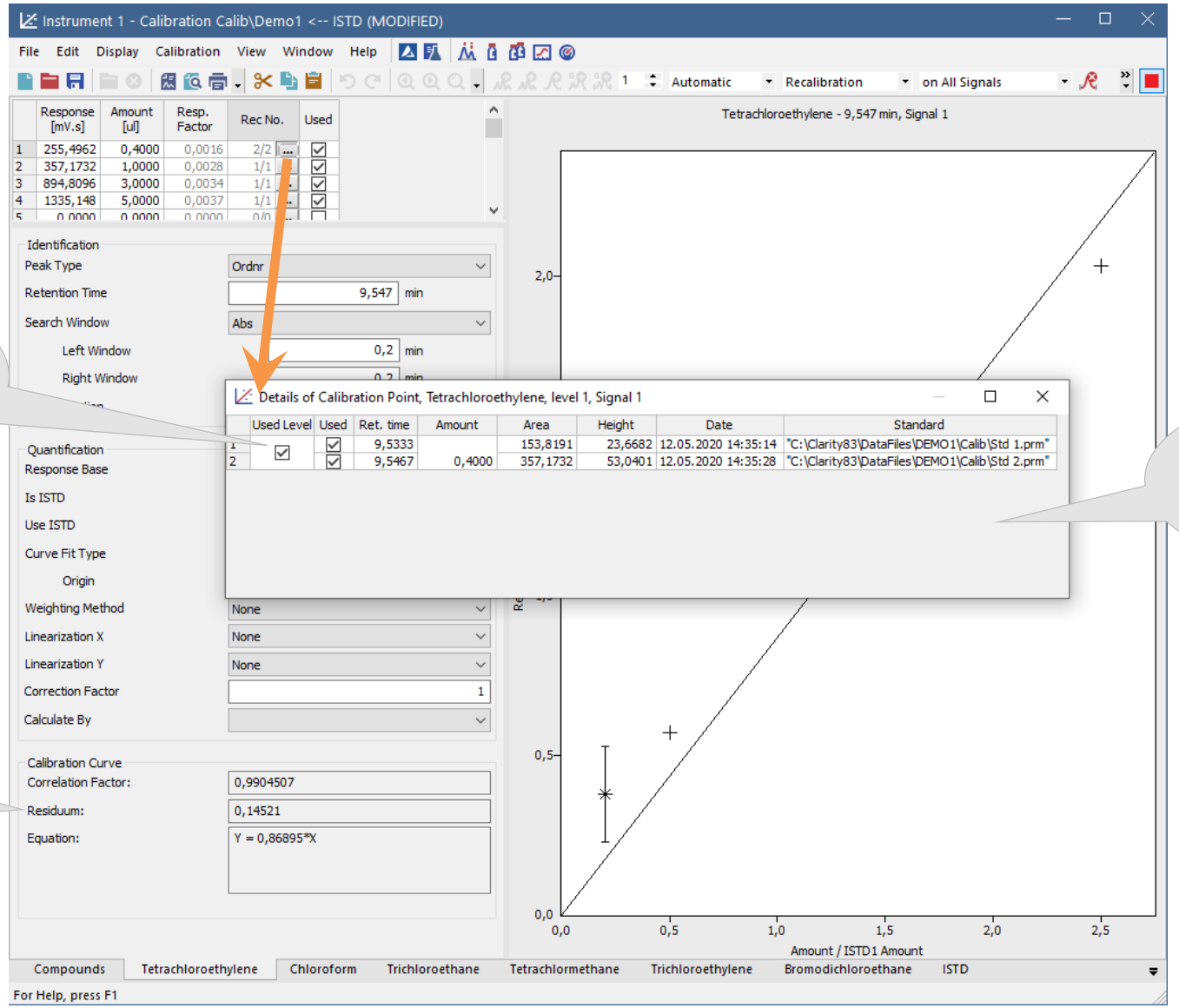
ADVANCED – PART 2

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

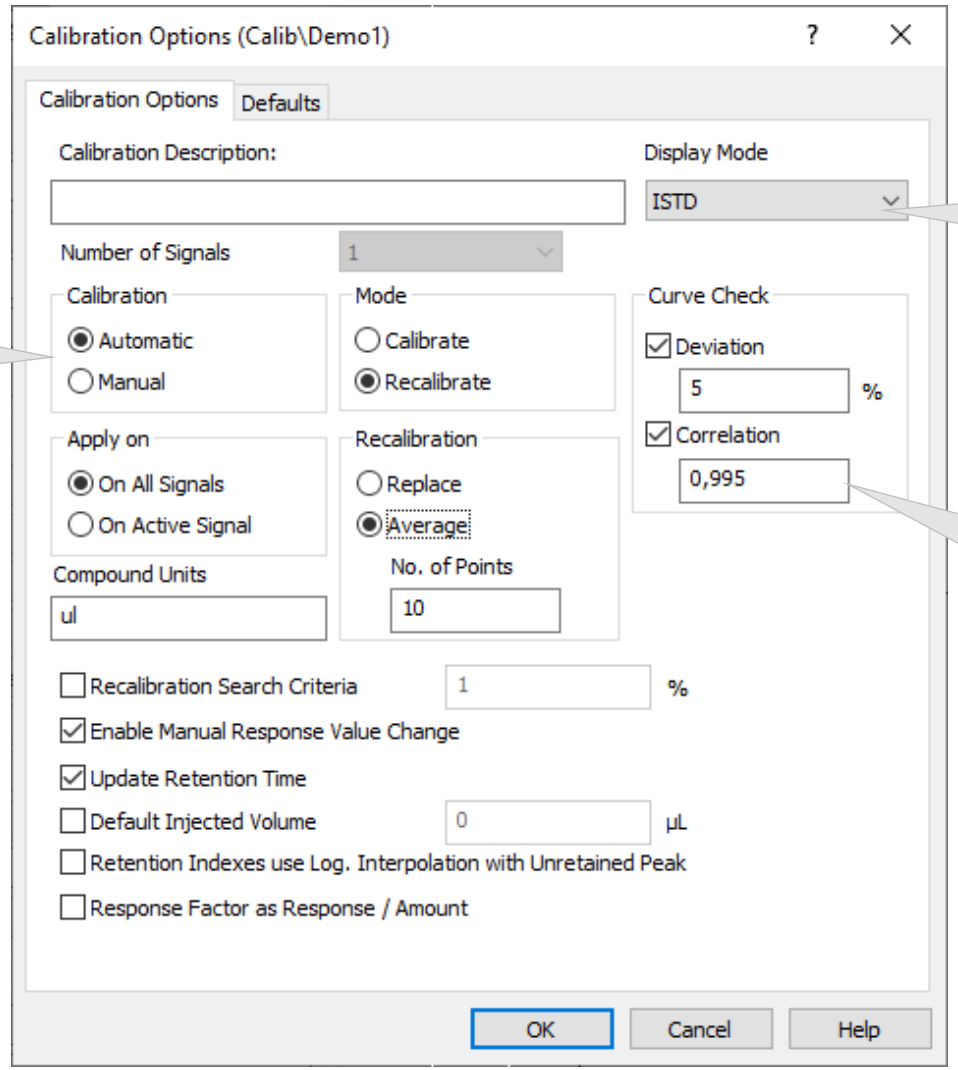


(Un)check checkbox to **include/omitt** from calibration

Menu Calibration / **Show Details** displays data used for selected level

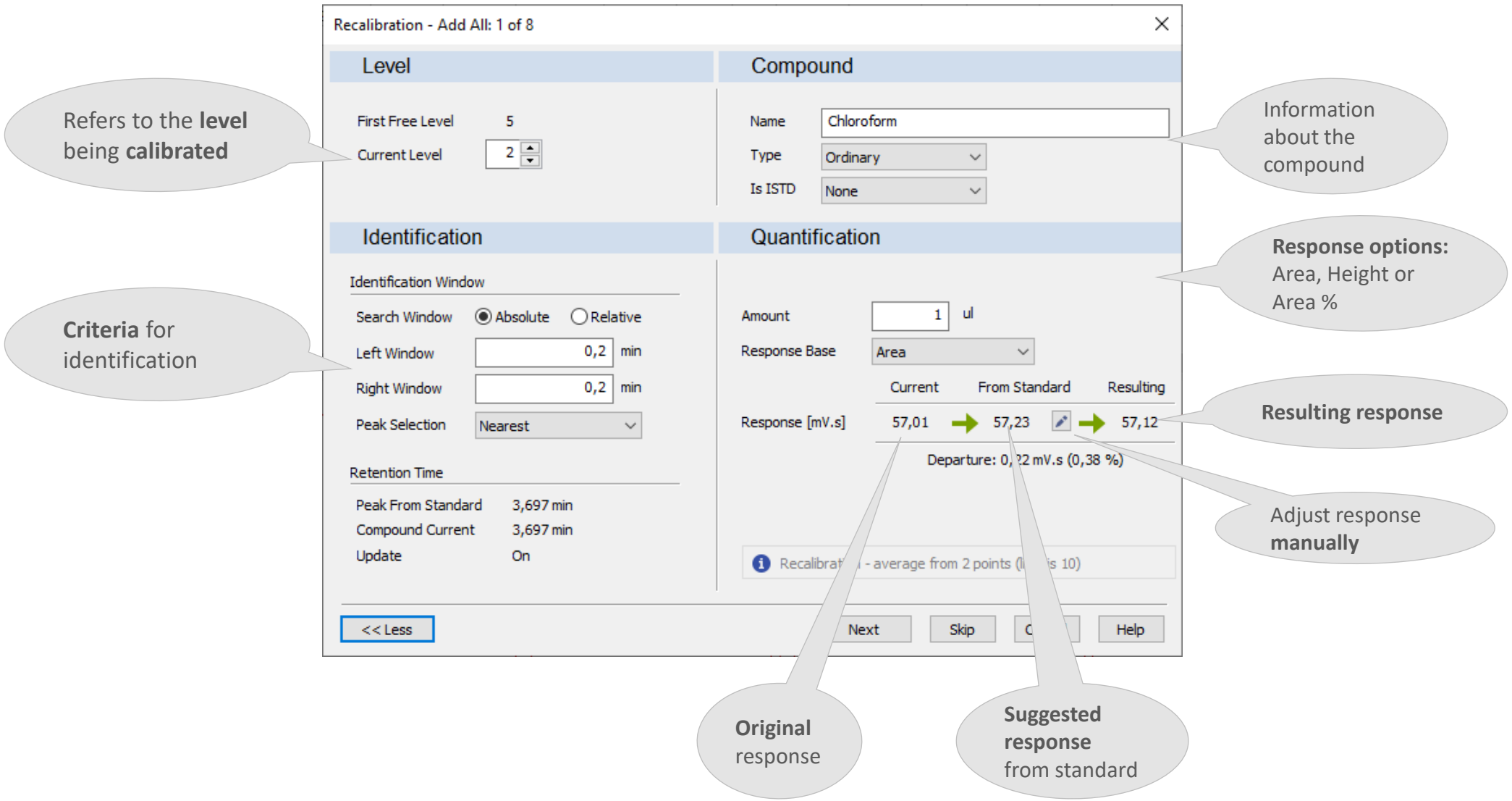
Residual sum of deviation squares

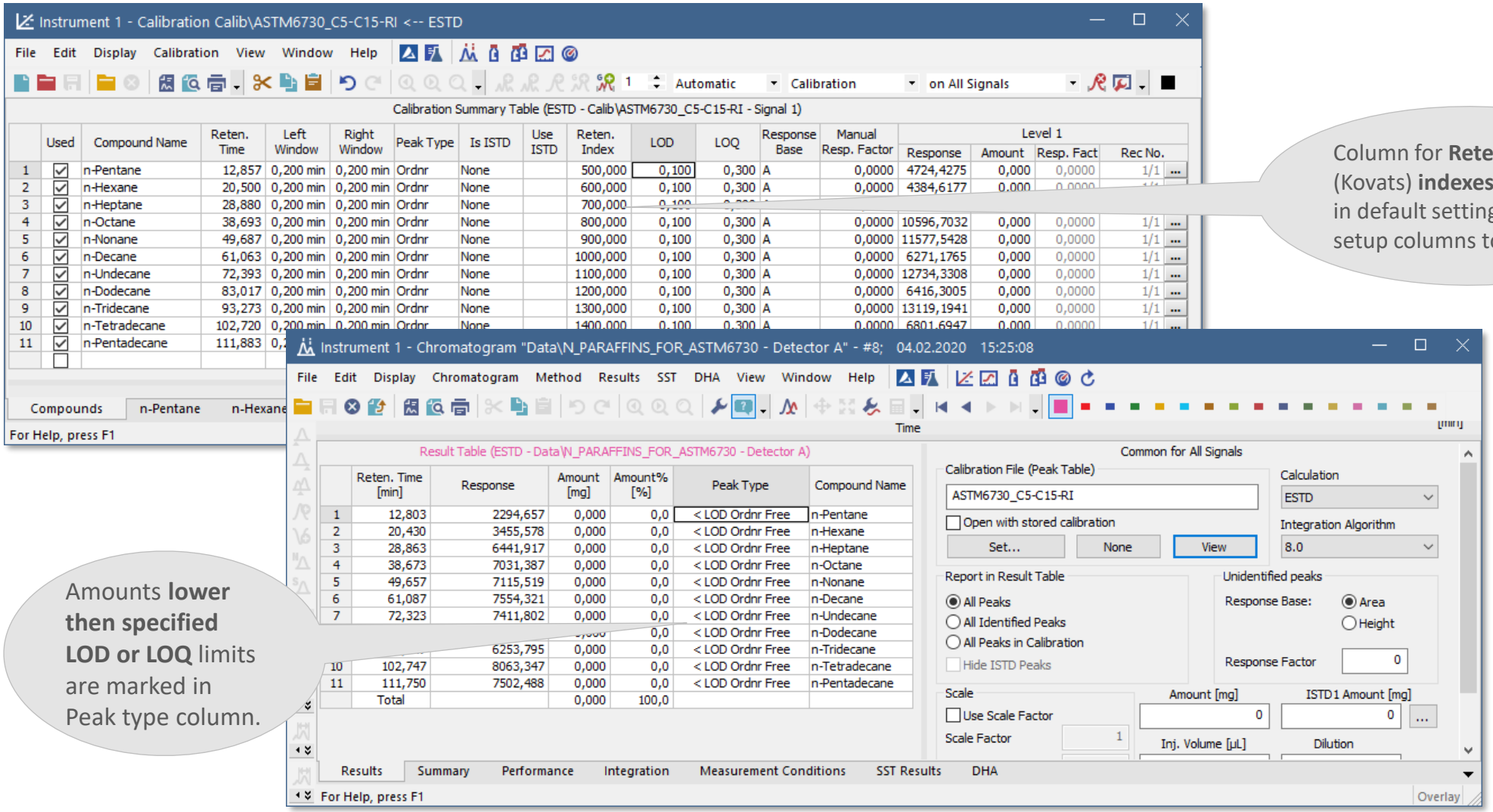
Refers to **automatic** or **manual** calibration



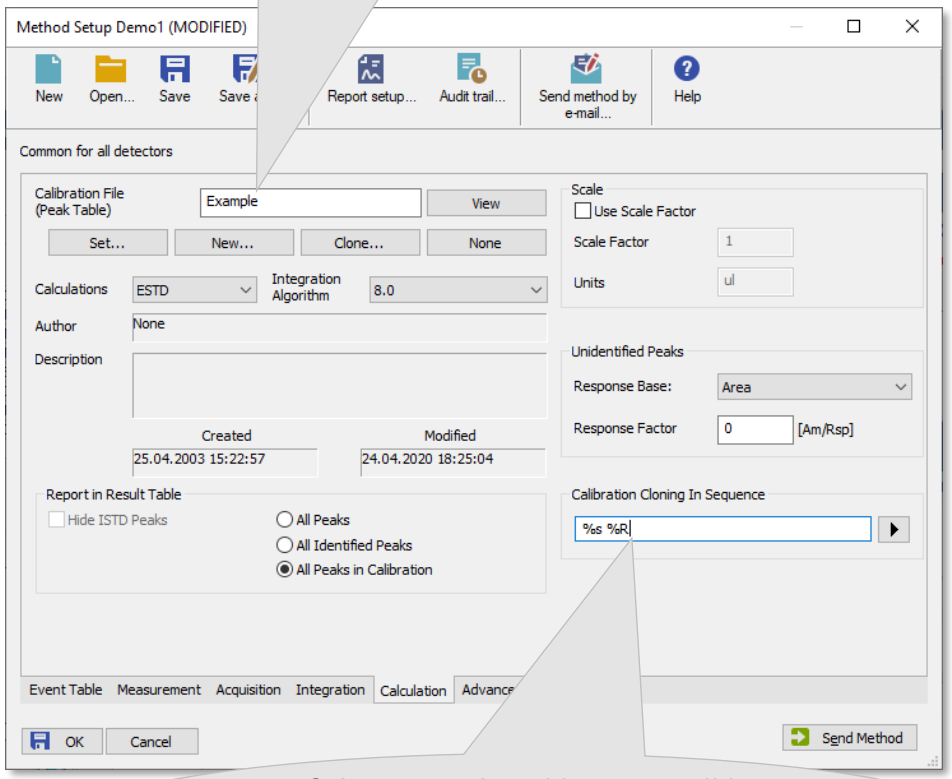
Calculation types: ESTD, ISTD, NORM, STDADD

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

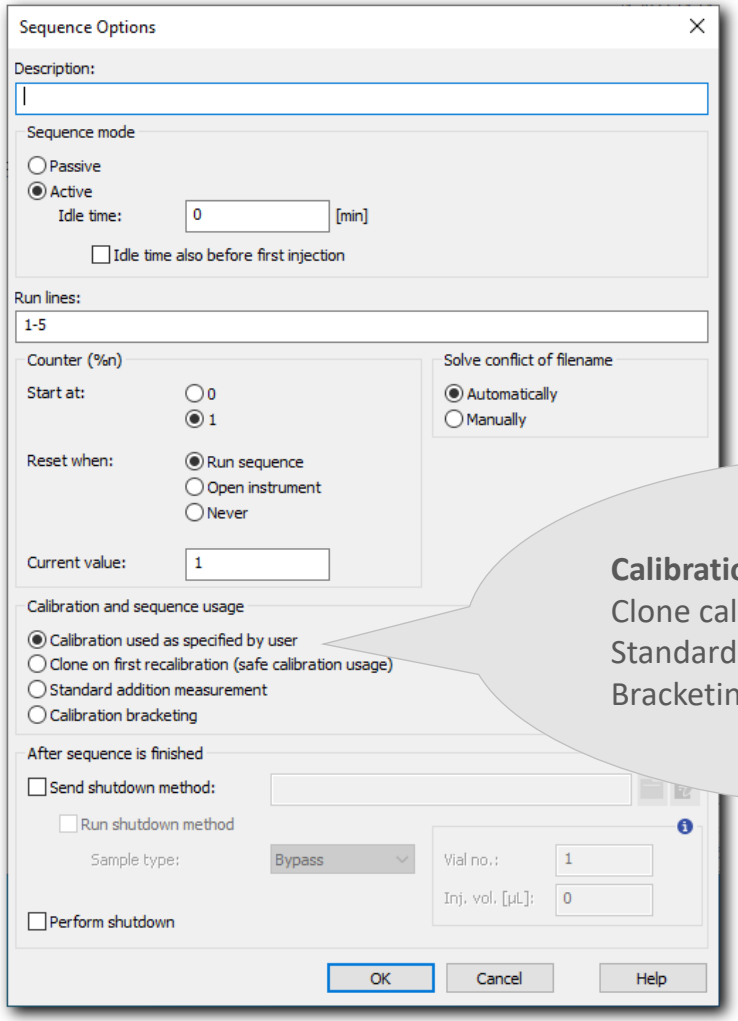

Recalibration - Add All: 1 of 8
Level
First Free Level 5
Current Level 2
Compound
Name Chloroform
Type Ordinary
Is ISTD None
Identification
Identification Window
Search Window Absolute Relative
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Retention Time
Peak From Standard 3,697 min
Compound Current 3,697 min
Update On
Quantification
Amount 1 ul
Response Base Area
Current From Standard Resulting
Response [mV.s] 57,01 57,23 57,12
Departure: 0,22 mV.s (0,38 %)
Recalibrat - average from 2 points (
s 10)
<< Less
Next
Skip
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


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 | Level 1 Amount | Level 1 Resp. Fact | Level 1 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 10596,7032 0,000 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 11577,5428 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 6271,1765 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 12734,3308 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 6416,3005 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 13119,1941 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 6801,6947 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
11 n-Pentadecane 111,883
Compounds n-Pentane n-Hexane
For Help, press F1
Column for Retention (Kovats) indexes is hidden in default settings. Use setup columns to display it.
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
Time
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 0,0 < LOD Ordnr Free n-Pentane
2 20,430 3455,578 0,000 0,0 < LOD Ordnr Free n-Hexane
3 28,863 6441,917 0,000 0,0 < LOD Ordnr Free n-Heptane
4 38,673 7031,387 0,000 0,0 < LOD Ordnr Free n-Octane
5 49,657 7115,519 0,000 0,0 < LOD Ordnr Free n-Nonane
6 61,087 7554,321 0,000 0,0 < LOD Ordnr Free n-Decane
7 72,323 7411,802 0,000 0,0 < LOD Ordnr Free n-Undecane
0,0 < LOD Ordnr Free n-Dodecane
6253,795 0,000 0,0 < LOD Ordnr Free n-Tridecane
10 102,747 8063,347 0,000 0,0 < LOD Ordnr Free n-Tetradecane
11 111,750 7502,488 0,000 0,0 < LOD Ordnr Free n-Pentadecane
Total 0,000 100,0
Common for All Signals
Calibration File (Peak Table)
ASTM6730_C5-C15-RI
Open with stored calibration
Set... None View
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
ISTD1 Amount [mg] 0
Inj. Volume [µL]
Dilution
Results Summary Performance Integration Measurement Conditions SST Results DHA
For Help, press F1
Overlay
Amounts lower then specified LOD or LOQ limits are marked in Peak type column.

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



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



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

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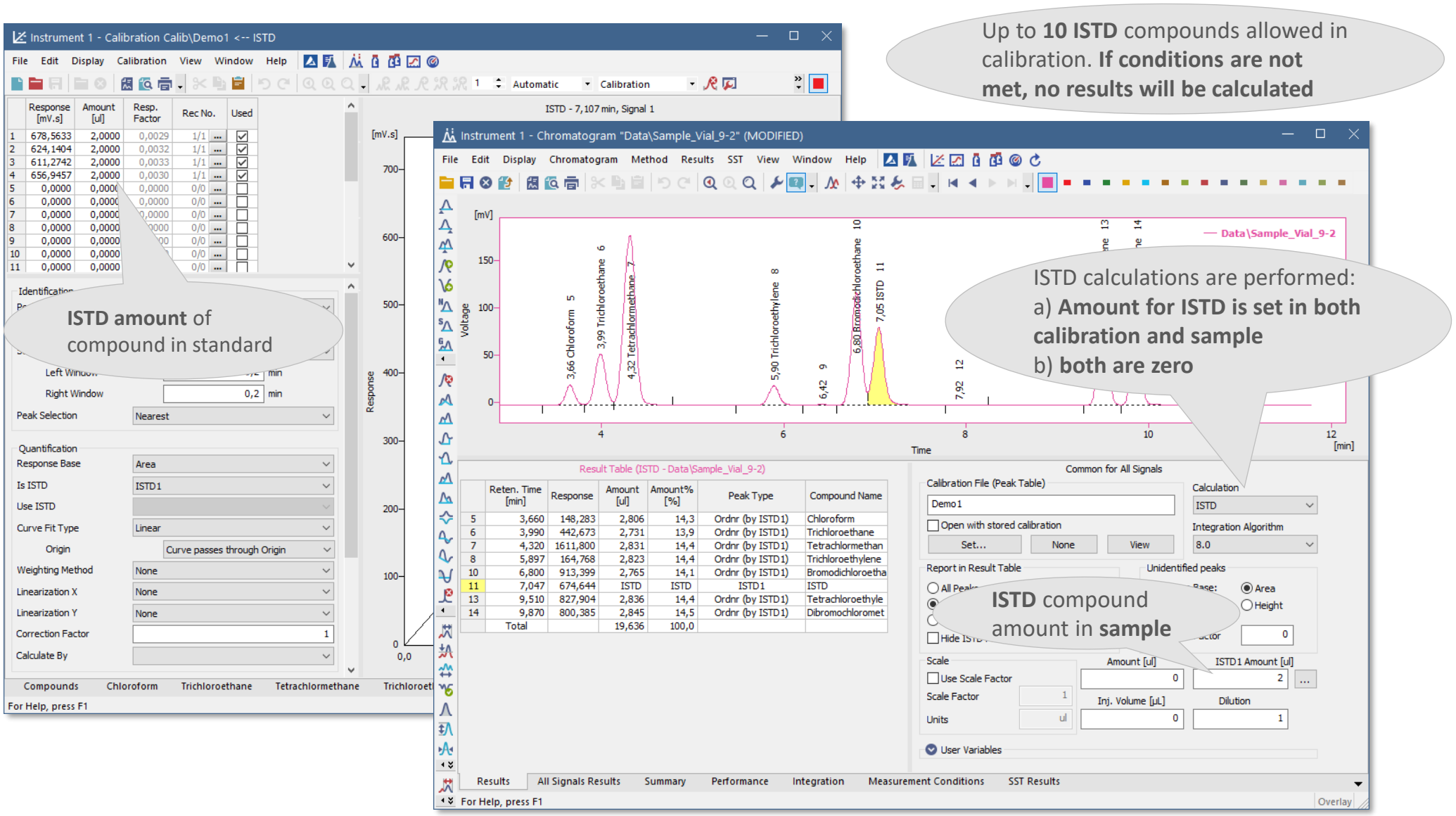
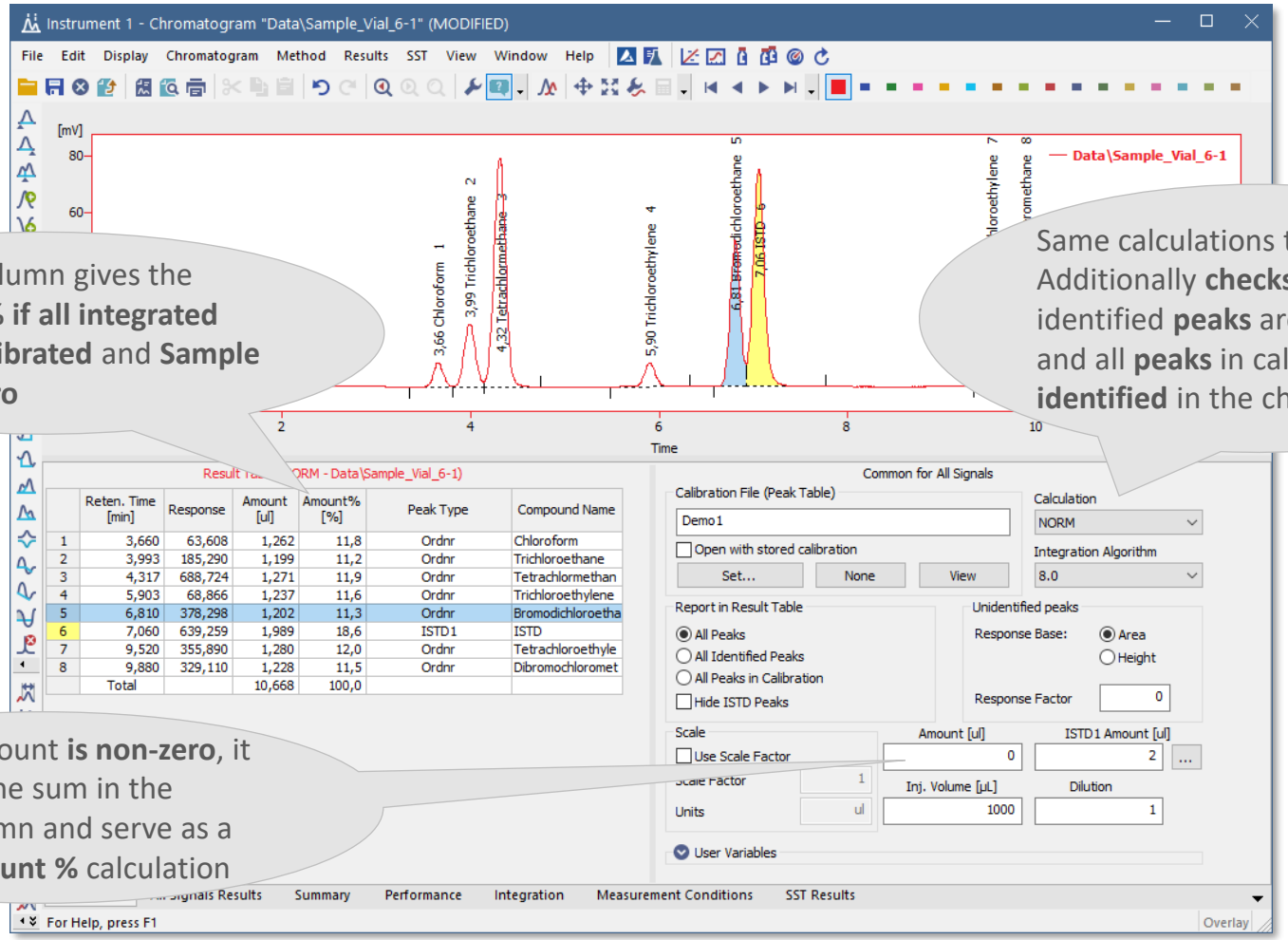

Up to **10 ISTD** compounds allowed in calibration. **If conditions are not met, no results will be calculated**
ISTD amount of compound in standard
ISTD calculations are performed:
a) **Amount for ISTD is set in both calibration and sample**
b) **both are zero**
ISTD compound amount in **sample**
Instrument 1 - Calibration Calib\Demo1 <-- ISTD
Instrument 1 - Chromatogram "Data\Sample_Vial_9-2" (MODIFIED)
Result Table (ISTD - Data\Sample_Vial_9-2)
Common for All Signals
Calibration File (Peak Table)
Demo 1
Calculation
ISTD
Integration Algorithm
8.0
Report in Result Table
Unidentified peaks
Scale
Use Scale Factor
Amount [ul]
ISTD1 Amount [ul]
Inj. Volume [µL]
Dilution
User Variables
Results
All Signals Results
Summary
Performance
Integration
Measurement Conditions
SST Results
For Help, press F1



	Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
1	3,660	63,608	1,262	11,8	Ordnr	Chloroform
2	3,993	185,290	1,199	11,2	Ordnr	Trichloroethane
3	4,317	688,724	1,271	11,9	Ordnr	Tetrachlormethan
4	5,903	68,866	1,237	11,6	Ordnr	Trichloroethylene
5	6,810	378,298	1,202	11,3	Ordnr	Bromodichloroetha
6	7,060	639,259	1,989	18,6	ISTD1	ISTD
7	9,520	355,890	1,280	12,0	Ordnr	Tetrachloroethyle
8	9,880	329,110	1,228	11,5	Ordnr	Dibromochloromet
	Total		10,668	100,0		

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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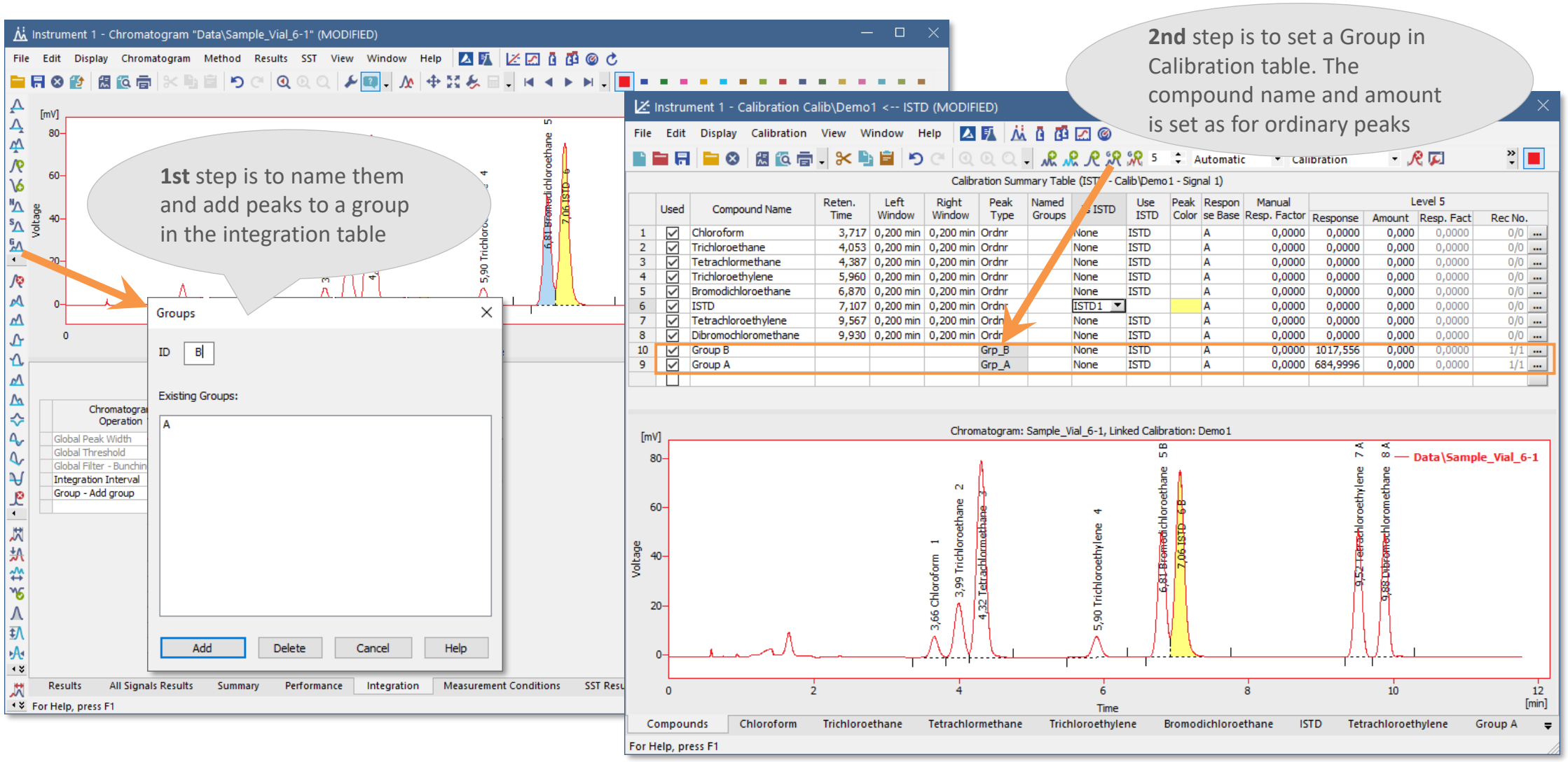
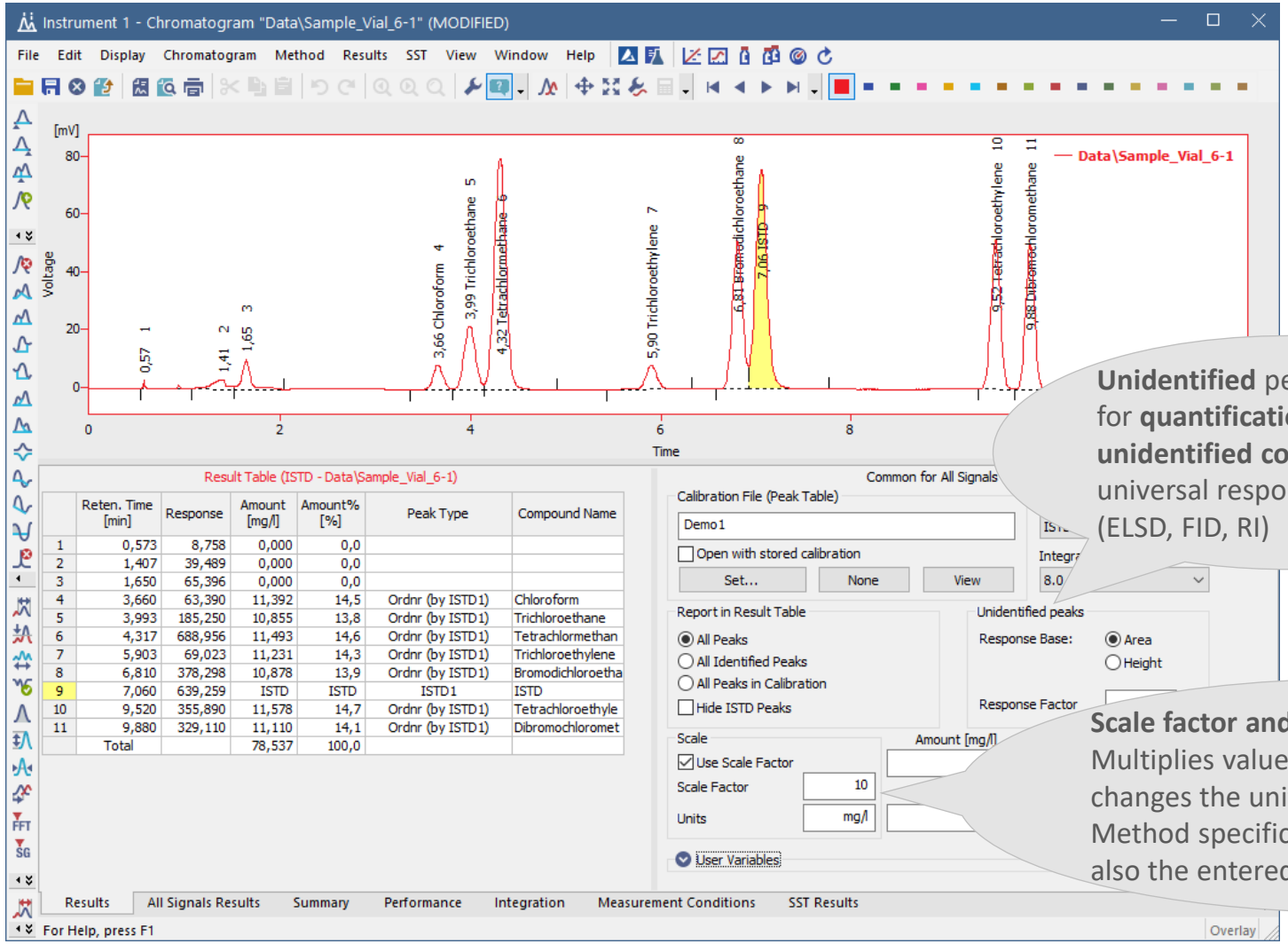
- Dilution
- Injection volume
  - Single analysis and calibration options
  - Autosampler in single run
- User variables


Instrument 1 - Chromatogram "Data\Sample_Vial_6-1" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
1st step is to name them and add peaks to a group in the integration table
Groups
ID B
Existing Groups:
A
Add Delete Cancel Help
Chromatogram Operation
Global Peak Width
Global Threshold
Global Filter - Bunchin
Integration Interval
Group - Add group
Results All Signals Results Summary Performance Integration Measurement Conditions SST Resu
For Help, press F1
2nd step is to set a Group in Calibration table. The compound name and amount is set as for ordinary peaks
Instrument 1 - Calibration Calib\Demo1 <-- ISTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
Calibration Summary Table (ISTD - Calib\Demo1 - Signal 1)
Used Compound Name Reten. Time Left Window Right Window Peak Type Named Groups ISTD Use ISTD Peak Color Response Base Manual Resp. Factor Level 5 Response Amount Resp. Fact Rec No.
1 Chloroform 3,717 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
2 Trichloroethane 4,053 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
3 Tetrachlormethane 4,387 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
4 Trichloroethylene 5,960 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
5 Bromodichloroethane 6,870 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
6 ISTD 7,107 0,200 min 0,200 min Ordnr ISTD1 A 0,0000 0,0000 0,000 0,0000 0/0
7 Tetrachloroethylene 9,567 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
8 Dibromochloromethane 9,930 0,200 min 0,200 min Ordnr None ISTD A 0,0000 0,0000 0,000 0,0000 0/0
10 Group B Grp_B None ISTD A 0,0000 1017,556 0,000 0,0000 1/1
9 Group A Grp_A None ISTD A 0,0000 684,9996 0,000 0,0000 1/1
Chromatogram: Sample_Vial_6-1, Linked Calibration: Demo1
Data\Sample_Vial_6-1
3,66 Chloroform 1
3,99 Trichloroethane 2
4,32 Tetrachlormethane 3
5,90 Trichloroethylene 4
6,81 Bromodichloroethane 5 B
7,06 ISTD 6 B
9,52 Tetrachloroethylene 7 A
9,88 Dibromochloromethane 8 A
Time [min]
Compounds Chloroform Trichloroethane Tetrachlormethane Trichloroethylene Bromodichloroethane ISTD Tetrachloroethylene Group A
For Help, press F1

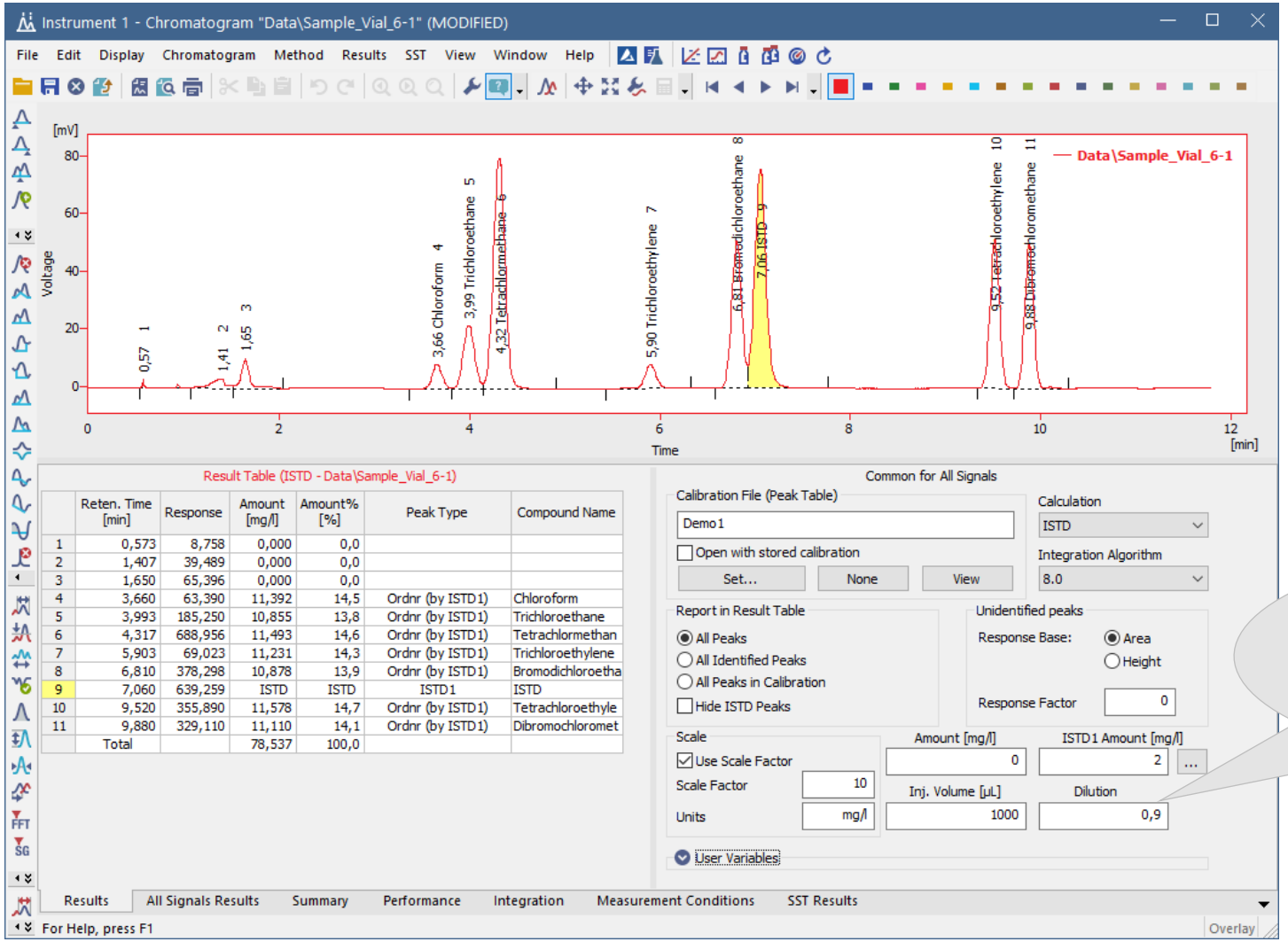
CHROMATOGRAM WINDOW → SCALE & UNCAL RESPONSE



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.

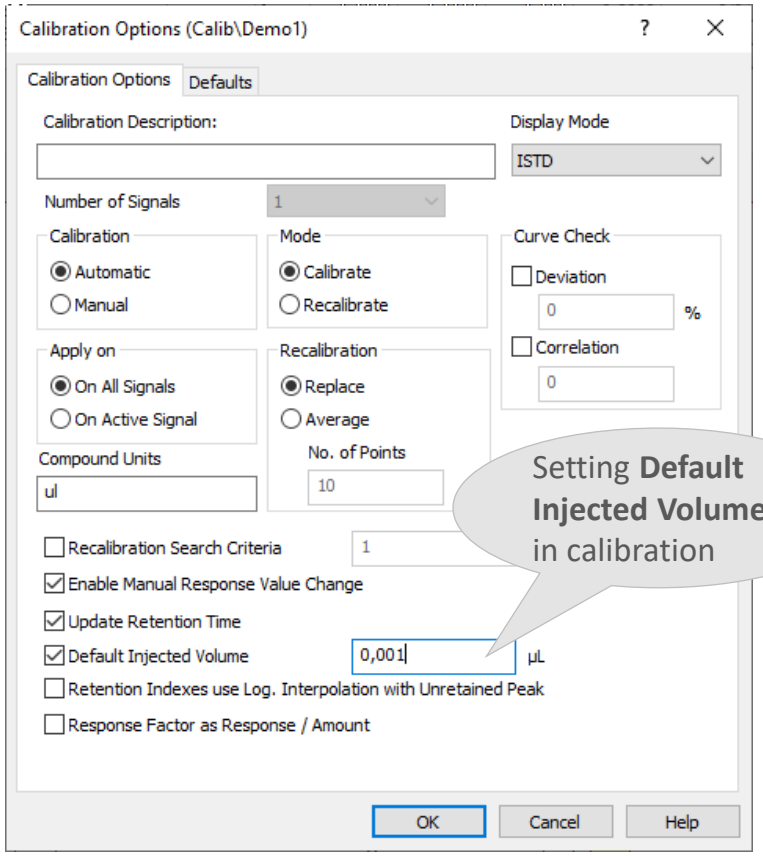
CHROMATOGRAM WINDOW → SCALE & UNCAL RESPONSE



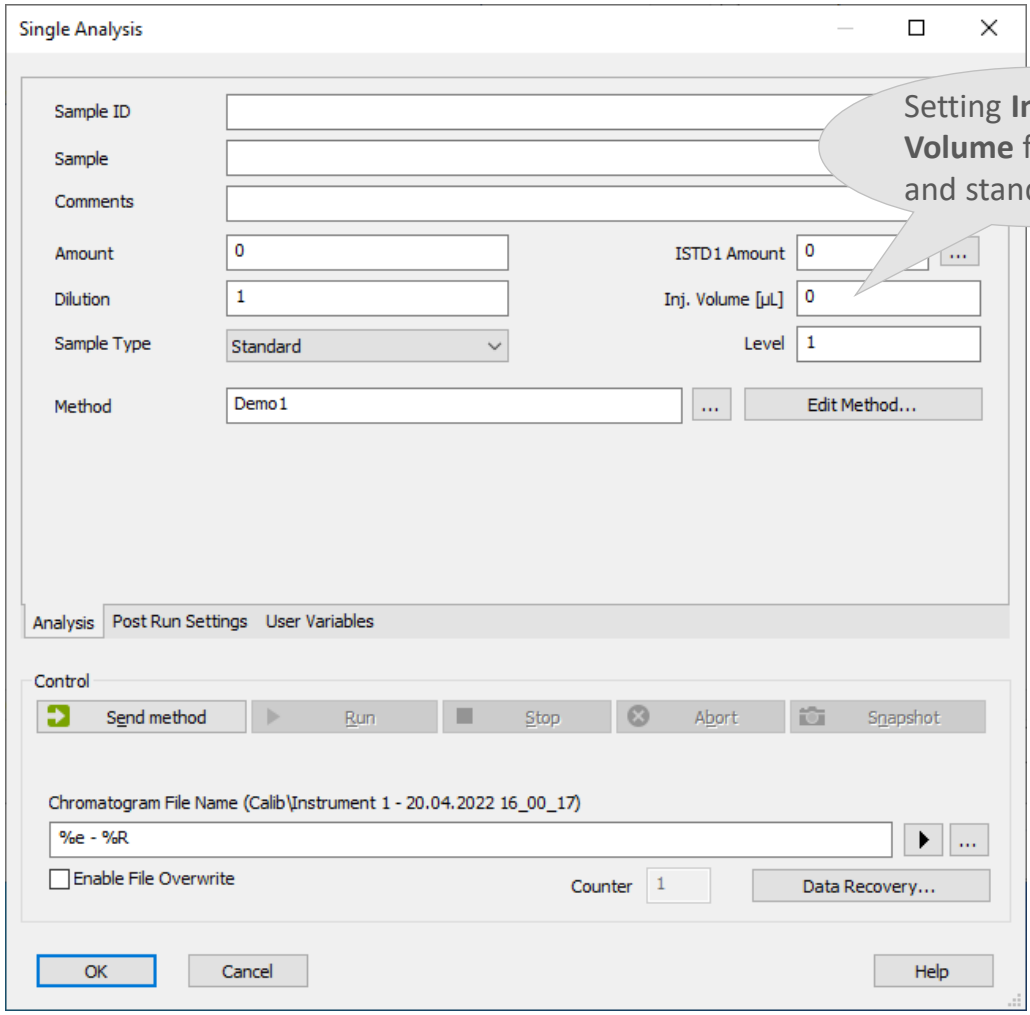
Dilution:
Multiplies values in Amount column. Sample specific parameter (entered from Sequence or Single Analysis window).

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

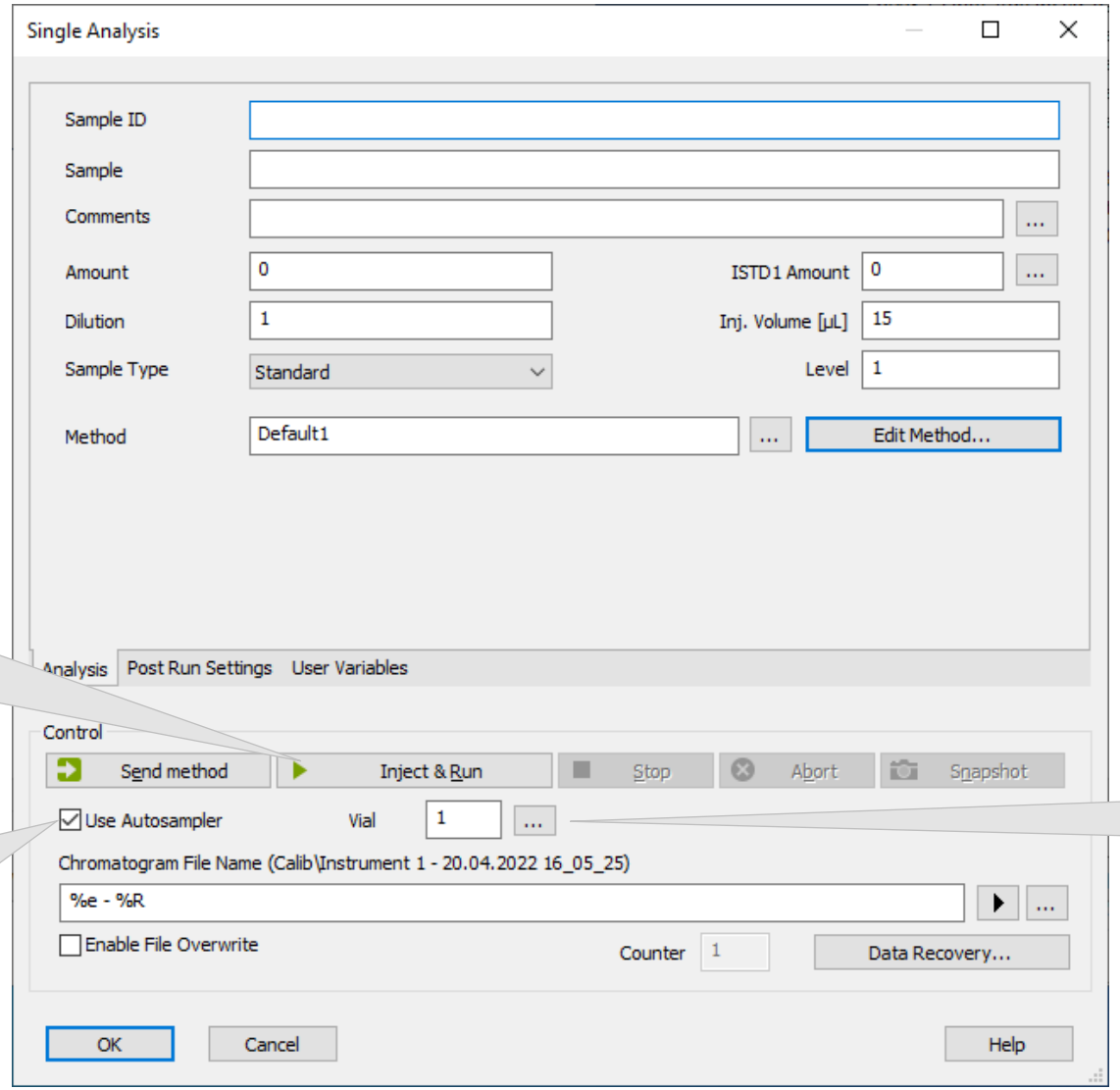
Supposes **linear detector** response
Improper use may lead to **incorrect results**



Setting **Default Injected Volume** in calibration



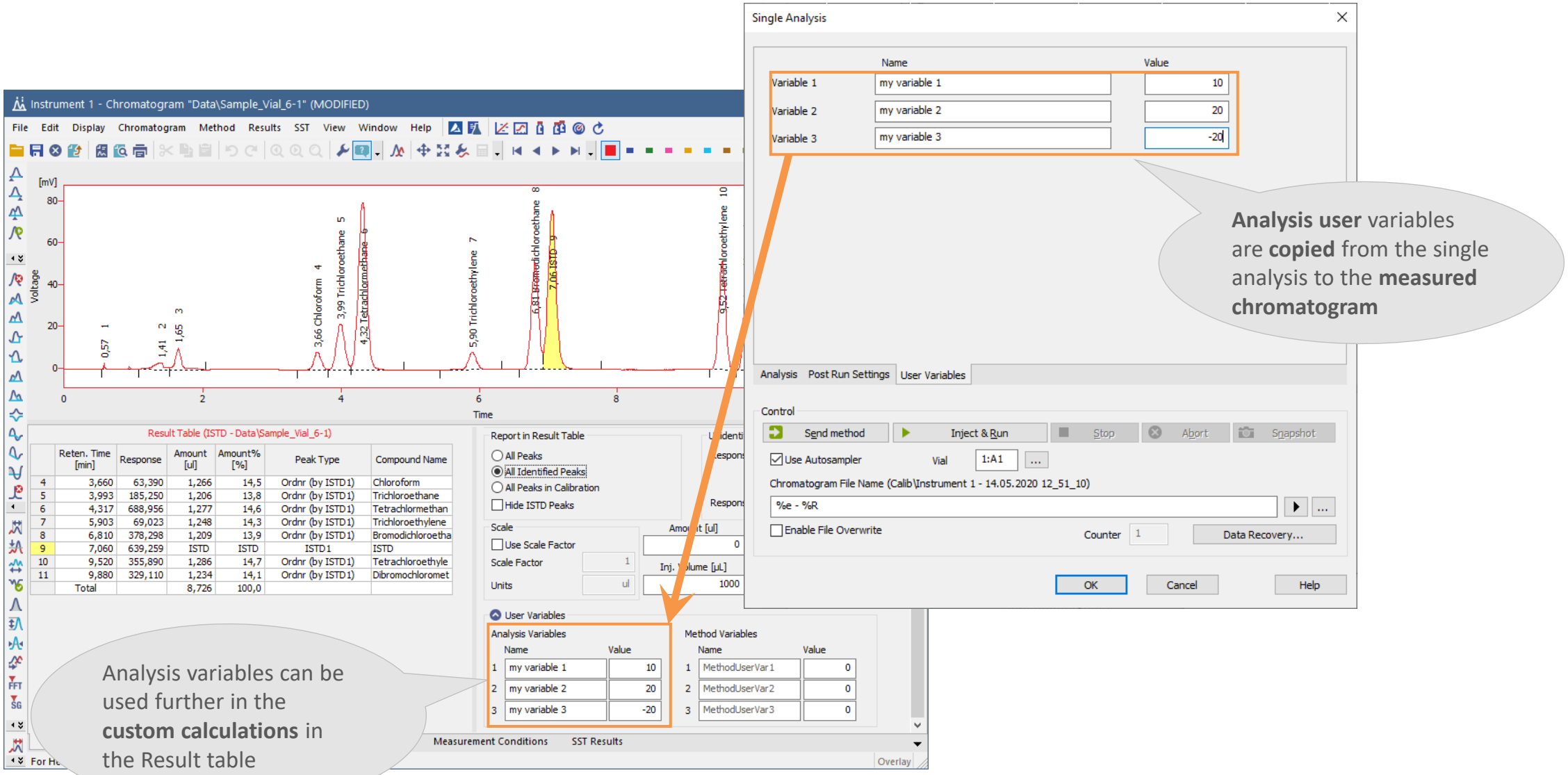
Setting **Injection Volume** for sample and standard



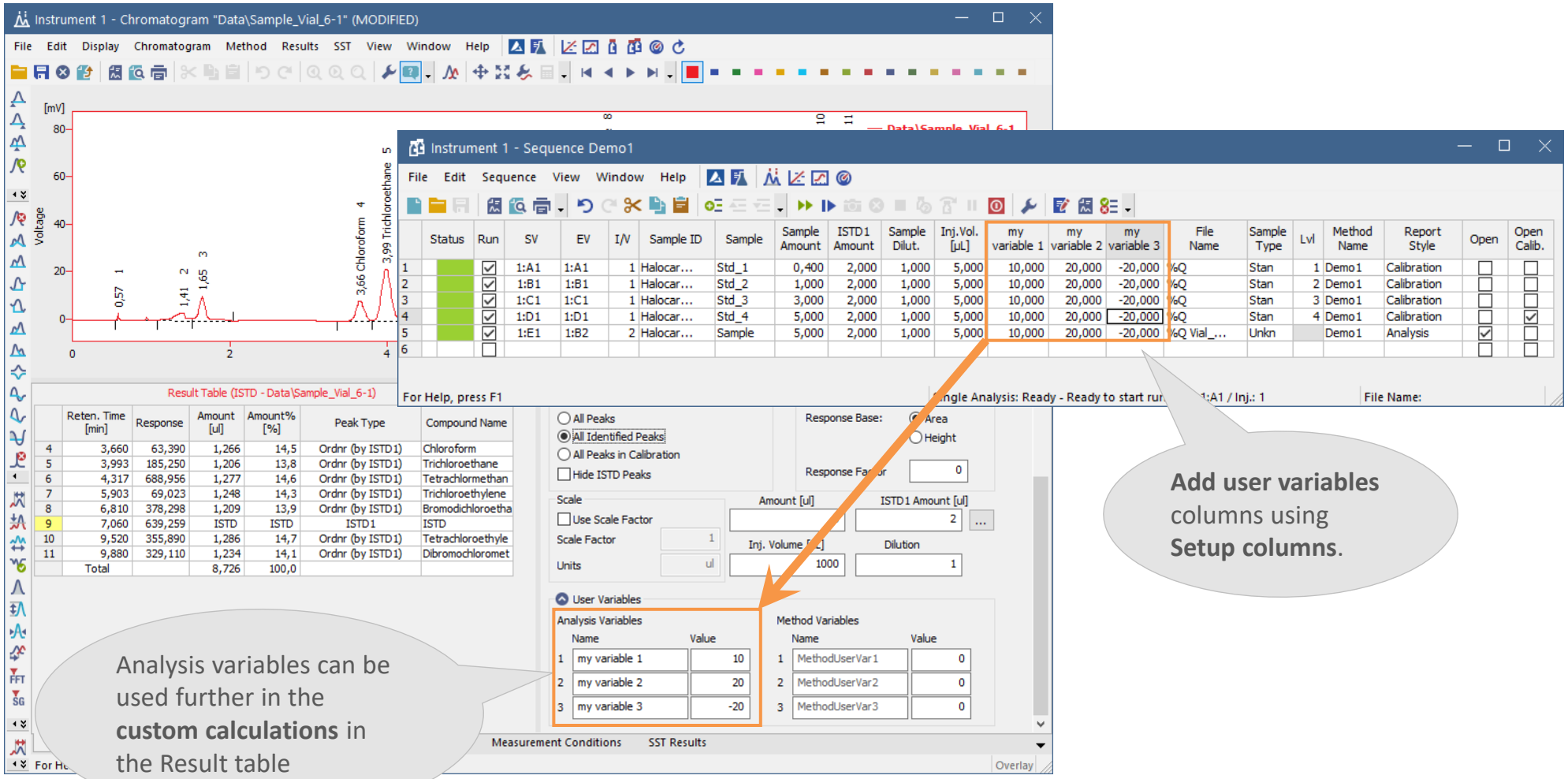
Perform one injection from the **specified Vial** and start the acquisition

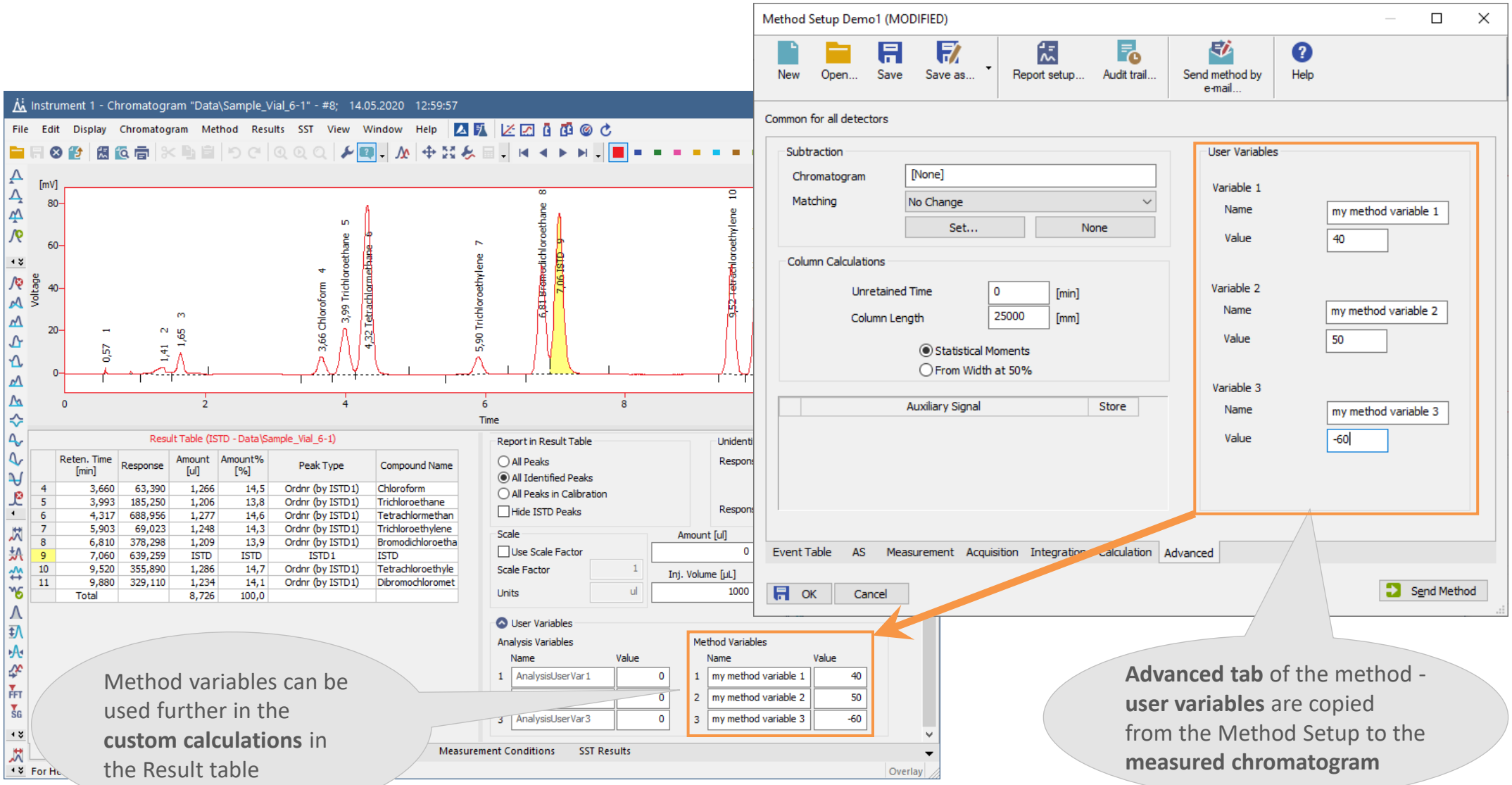
Use Autosampler – option **enabled** only if AS is configured on the instrument

Support for **graphical entry** of vial number


Single Analysis
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:A1
Chromatogram File Name (Calib\Instrument 1 - 14.05.2020 12_51_10)
%e - %R
Enable File Overwrite
Counter
Data Recovery...
OK
Cancel
Help
Analysis user variables are copied from the single analysis to the measured chromatogram
Instrument 1 - Chromatogram "Data\Sample_Vial_6-1" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
Time
0,57
1,41
1,65
3,66 Chloroform
3,99 Trichloroethane
4,32 Tetrachloromethane
5,90 Trichloroethylene
6,81 Bromodichloroethane
7,06 ISTD
9,52 Tetrachloroethylene
Result Table (ISTD - Data\Sample_Vial_6-1)
Reten. Time [min]
Response
Amount [ul]
Amount% [%]
Peak Type
Compound Name
4 3,660 63,390 1,266 14,5 Ordnr (by ISTD1) Chloroform
5 3,993 185,250 1,206 13,8 Ordnr (by ISTD1) Trichloroethane
6 4,317 688,956 1,277 14,6 Ordnr (by ISTD1) Tetrachlormethan
7 5,903 69,023 1,248 14,3 Ordnr (by ISTD1) Trichloroethylene
8 6,810 378,298 1,209 13,9 Ordnr (by ISTD1) Bromodichloroetha
9 7,060 639,259 ISTD ISTD ISTD1 ISTD
10 9,520 355,890 1,286 14,7 Ordnr (by ISTD1) Tetrachloroethyle
11 9,880 329,110 1,234 14,1 Ordnr (by ISTD1) Dibromochloromet
Total 8,726 100,0
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Hide ISTD Peaks
Scale
Use Scale Factor
Scale Factor
Units
User Variables
Analysis Variables
Name
Value
1 my variable 1 10
2 my variable 2 20
3 my variable 3 -20
Method Variables
1 MethodUserVar1 0
2 MethodUserVar2 0
3 MethodUserVar3 0
Measurement Conditions
SST Results
Overlay
Analysis variables can be used further in the custom calculations in the Result table

SEQUENCE → USER VARIABLES




Method Setup Demo1 (MODIFIED)
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
[min]
Column Length
25000
[mm]
Statistical Moments
From Width at 50%
Auxiliary Signal
Store
User Variables
Variable 1
Name
my method variable 1
Value
40
Variable 2
Name
my method variable 2
Value
50
Variable 3
Name
my method variable 3
Value
-60
Event Table
AS
Measurement
Acquisition
Integration
Calculation
Advanced
OK
Cancel
Send Method
Instrument 1 - Chromatogram "Data\Sample_Vial_6-1" - #8; 14.05.2020 12:59:57
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
Time
0,57 1
1,41 2
1,65 3
3,66 Chloroform 4
3,99 Trichloroethane 5
4,32 Tetrachlormethane 6
5,90 Trichloroethylene 7
6,81 Bromodichloroethane 8
7,06 ISTD 9
9,52 Tetrachloroethylene 10
Result Table (ISTD - Data\Sample_Vial_6-1)
Reten. Time [min]
Response
Amount [ul]
Amount% [%]
Peak Type
Compound Name
4 3,660 63,390 1,266 14,5 Ordnr (by ISTD1) Chloroform
5 3,993 185,250 1,206 13,8 Ordnr (by ISTD1) Trichloroethane
6 4,317 688,956 1,277 14,6 Ordnr (by ISTD1) Tetrachlormethan
7 5,903 69,023 1,248 14,3 Ordnr (by ISTD1) Trichloroethylene
8 6,810 378,298 1,209 13,9 Ordnr (by ISTD1) Bromodichloroetha
9 7,060 639,259 ISTD ISTD ISTD1 ISTD
10 9,520 355,890 1,286 14,7 Ordnr (by ISTD1) Tetrachloroethyle
11 9,880 329,110 1,234 14,1 Ordnr (by ISTD1) Dibromochloromet
Total 8,726 100,0
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Hide ISTD Peaks
Scale
Use Scale Factor
Scale Factor
Units
Amount [ul]
Inj. Volume [µL]
1000
User Variables
Analysis Variables
Name
Value
AnalysisUserVar1
AnalysisUserVar3
Method Variables
my method variable 1 40
my method variable 2 50
my method variable 3 -60
Measurement Conditions
SST Results
Overlay
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**

DataApex

SMART SOLUTION FOR LABORATORIES

...THANK YOU FOR YOUR TIME

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