DataApex

SMART SOLUTION FOR LABORATORIES

Clarity™

advanced chromatography software

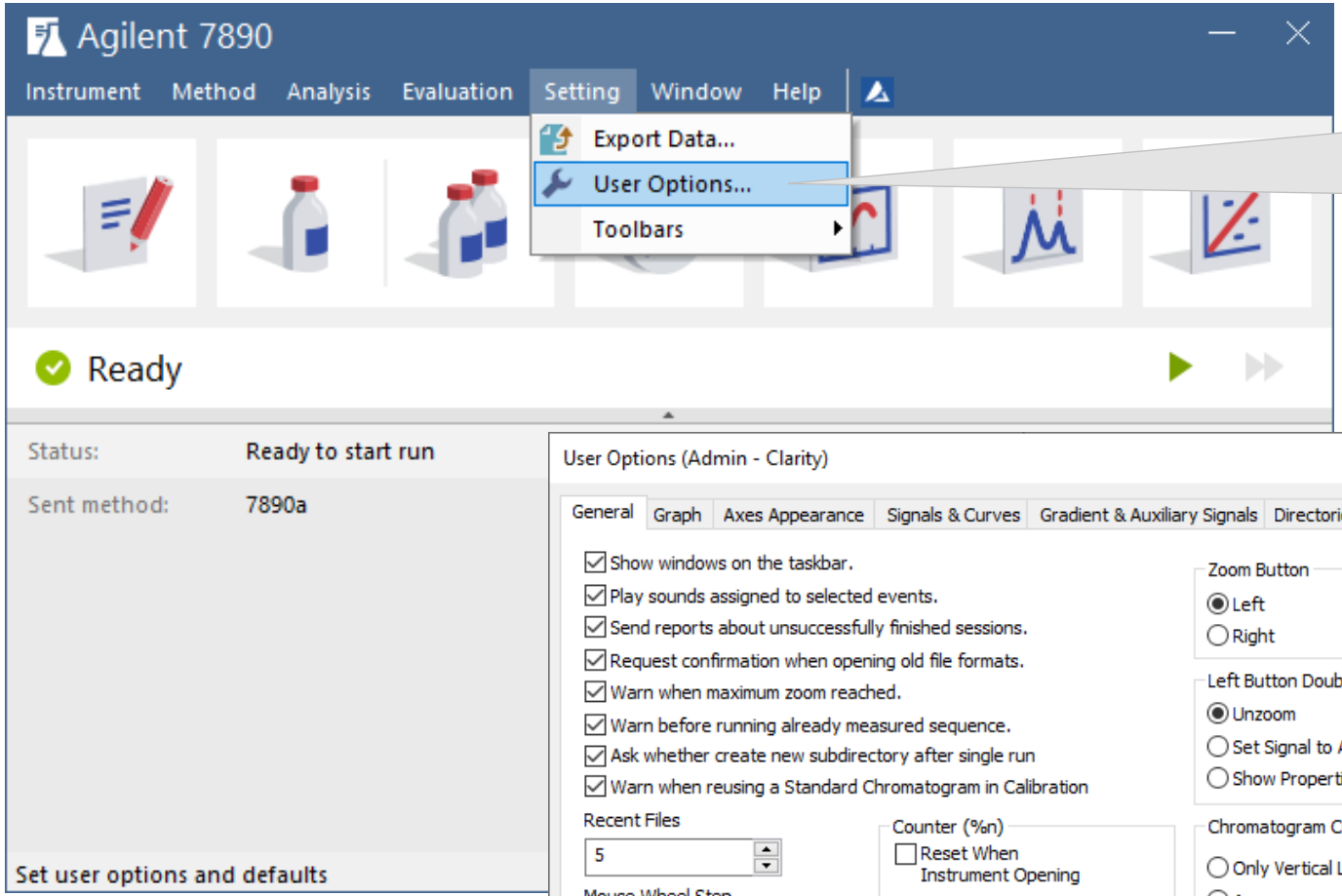
USER TRAINING

ADVANCED – PART 1

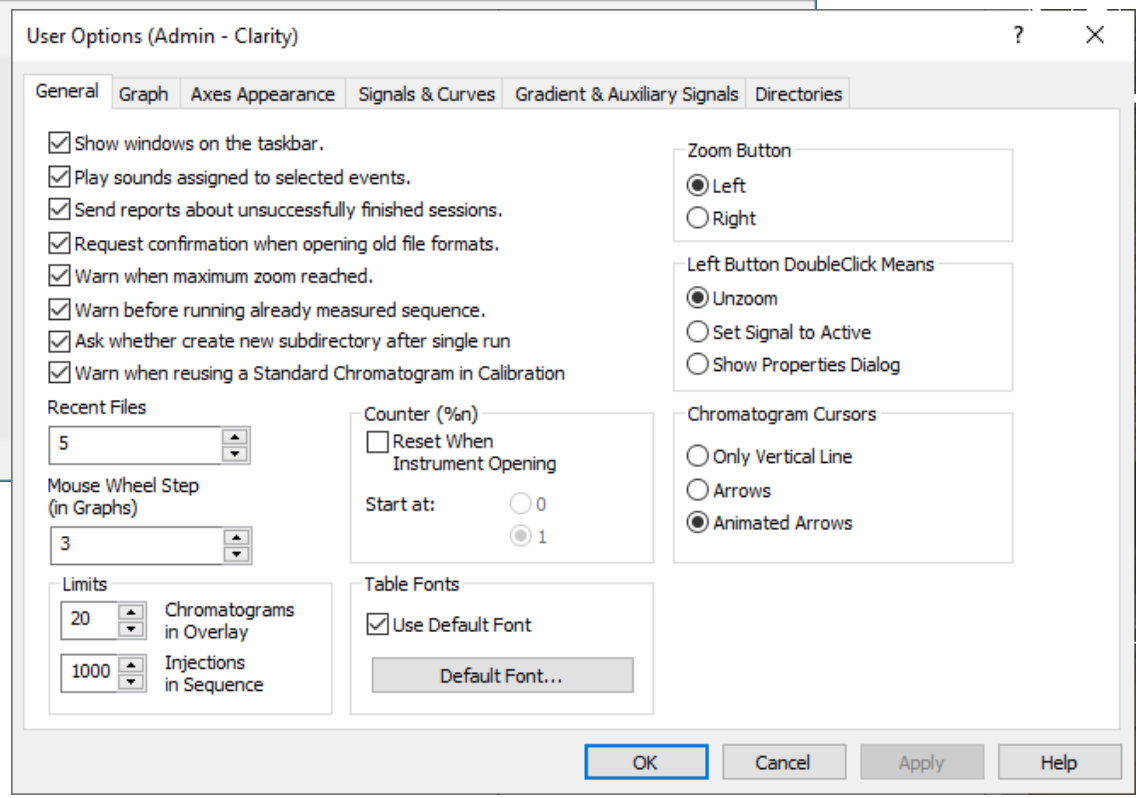
P008/80D 04/2022

Agenda

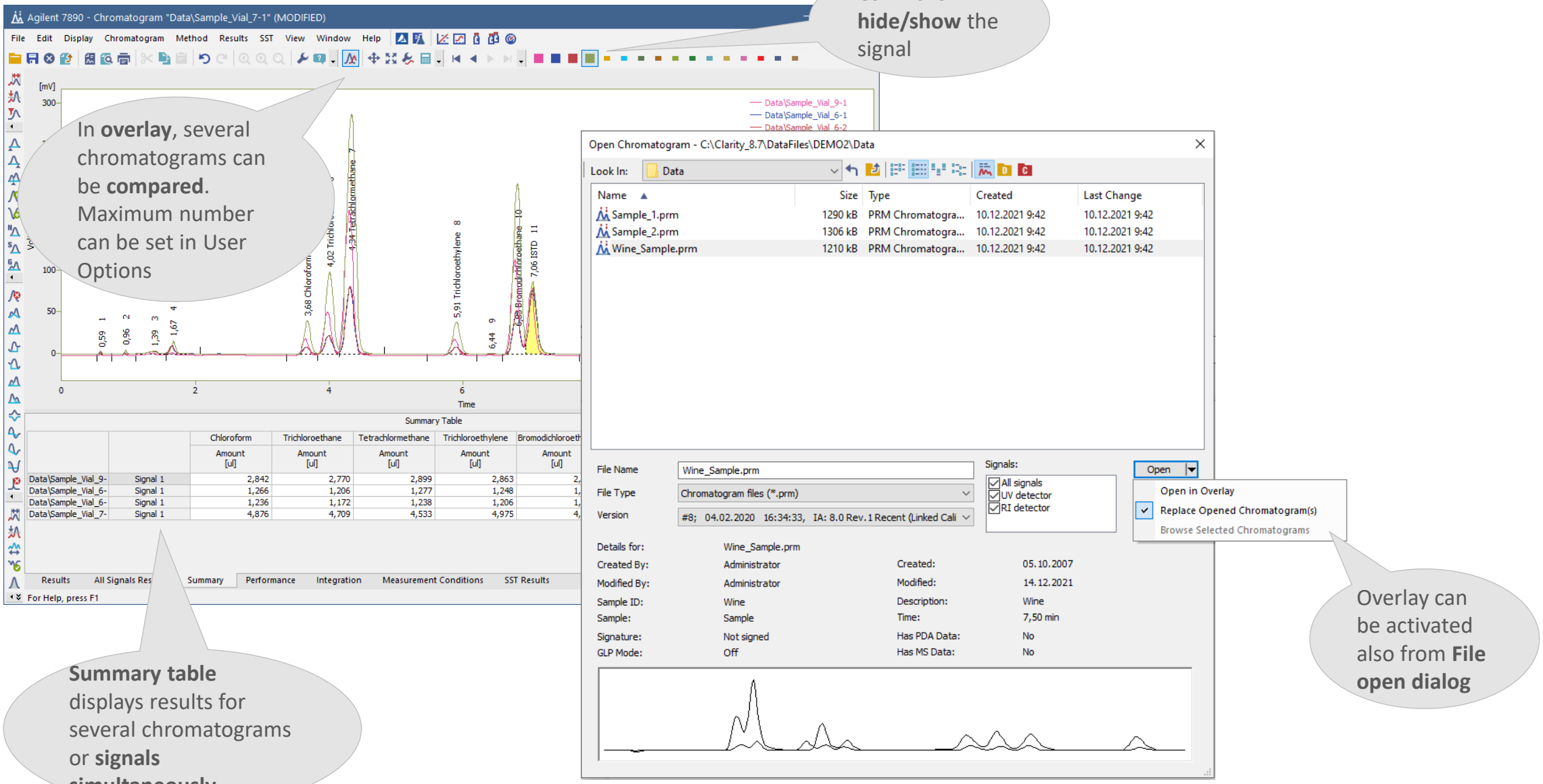
- Instrument window
- Chromatogram window
  - Overlay, 3D View and Labels
  - Setup columns
  - User columns
  - Noise and Drift
  - Performance tab
  - Force peak function
  - Peak coloring
  - Graph properties
- Sequence table
  - Overview
  - Description of sequence window
  - Basic functions
  - Sequence mode
  - Options
  - Import
  - Fill Series function



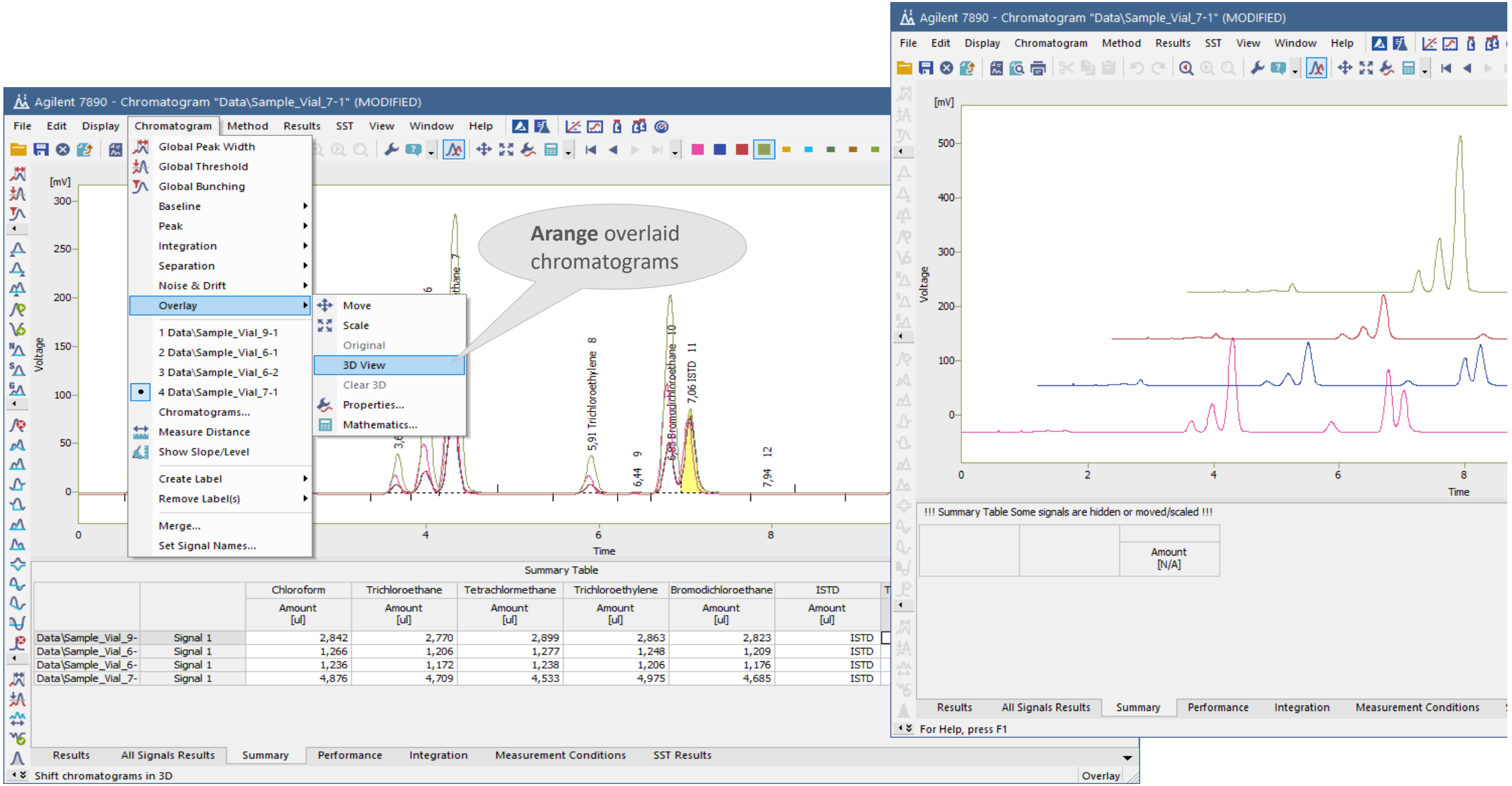
User settings are stored in individual users desktop ***.dsk** files.
For this reason they are set in the instrument window and not in the main Clarity window



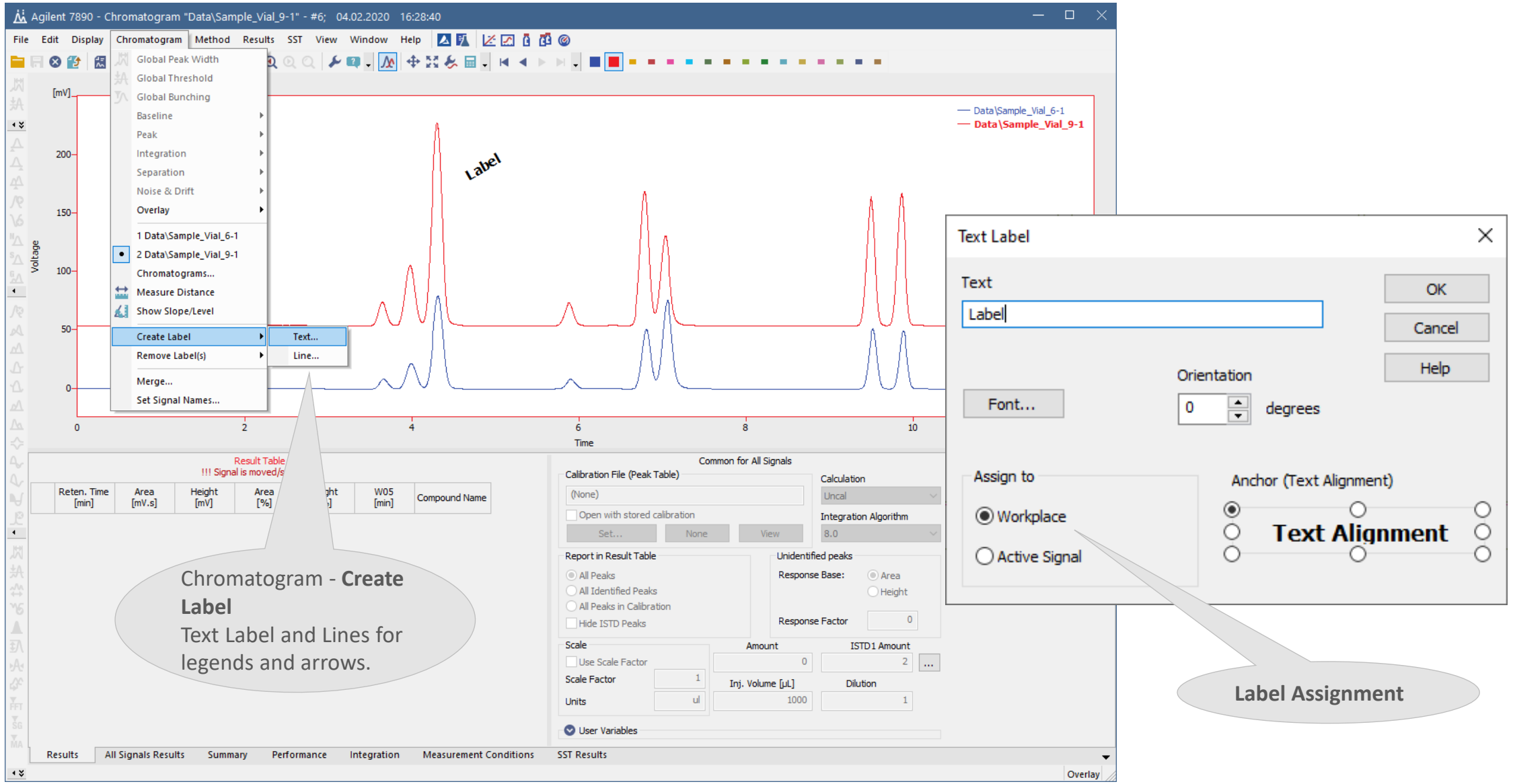
CHROMATOGRAM WINDOW → OVERLAY

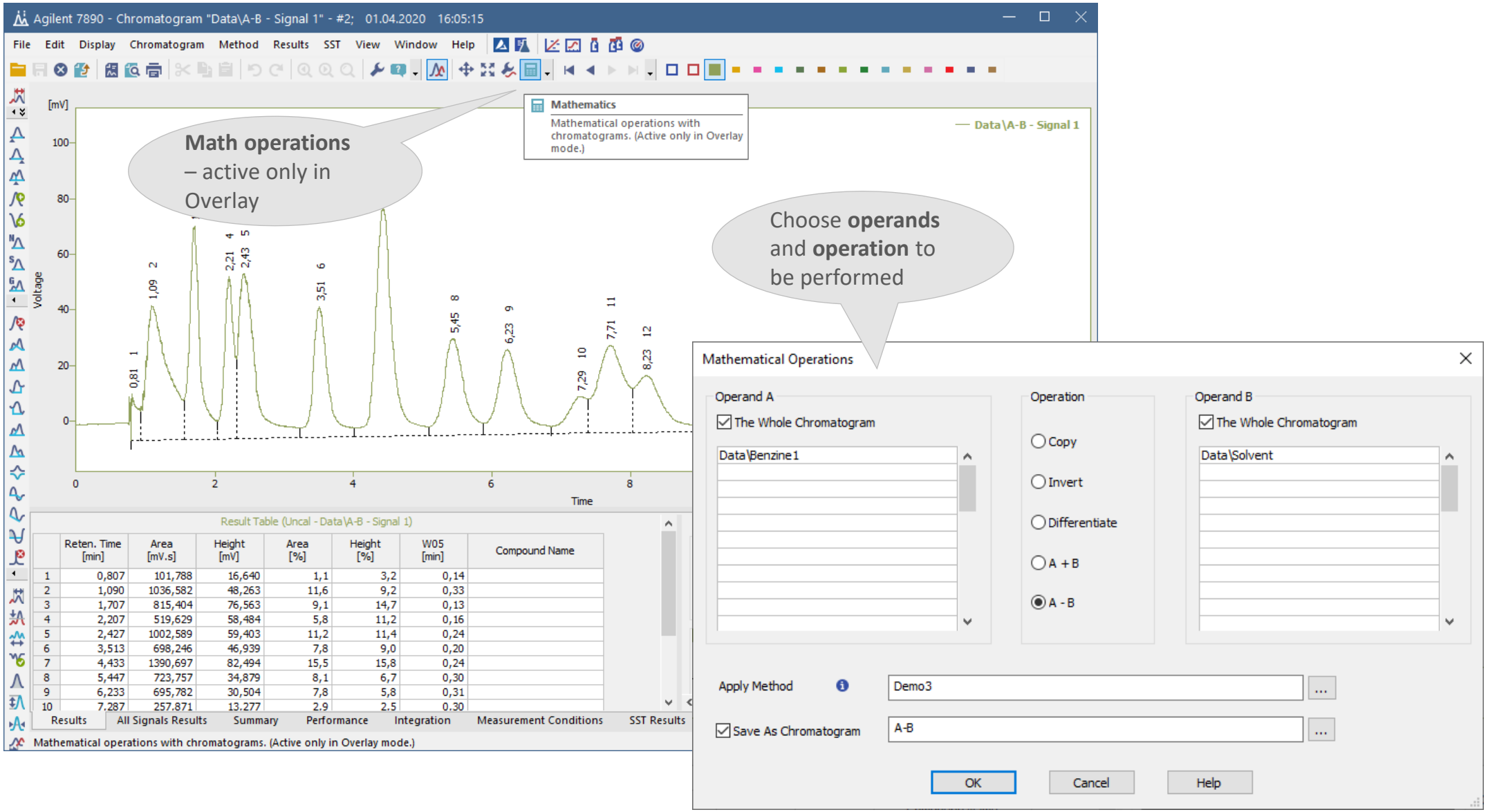


CHROMATOGRAM WINDOW → OVERLAY - 3D VIEW

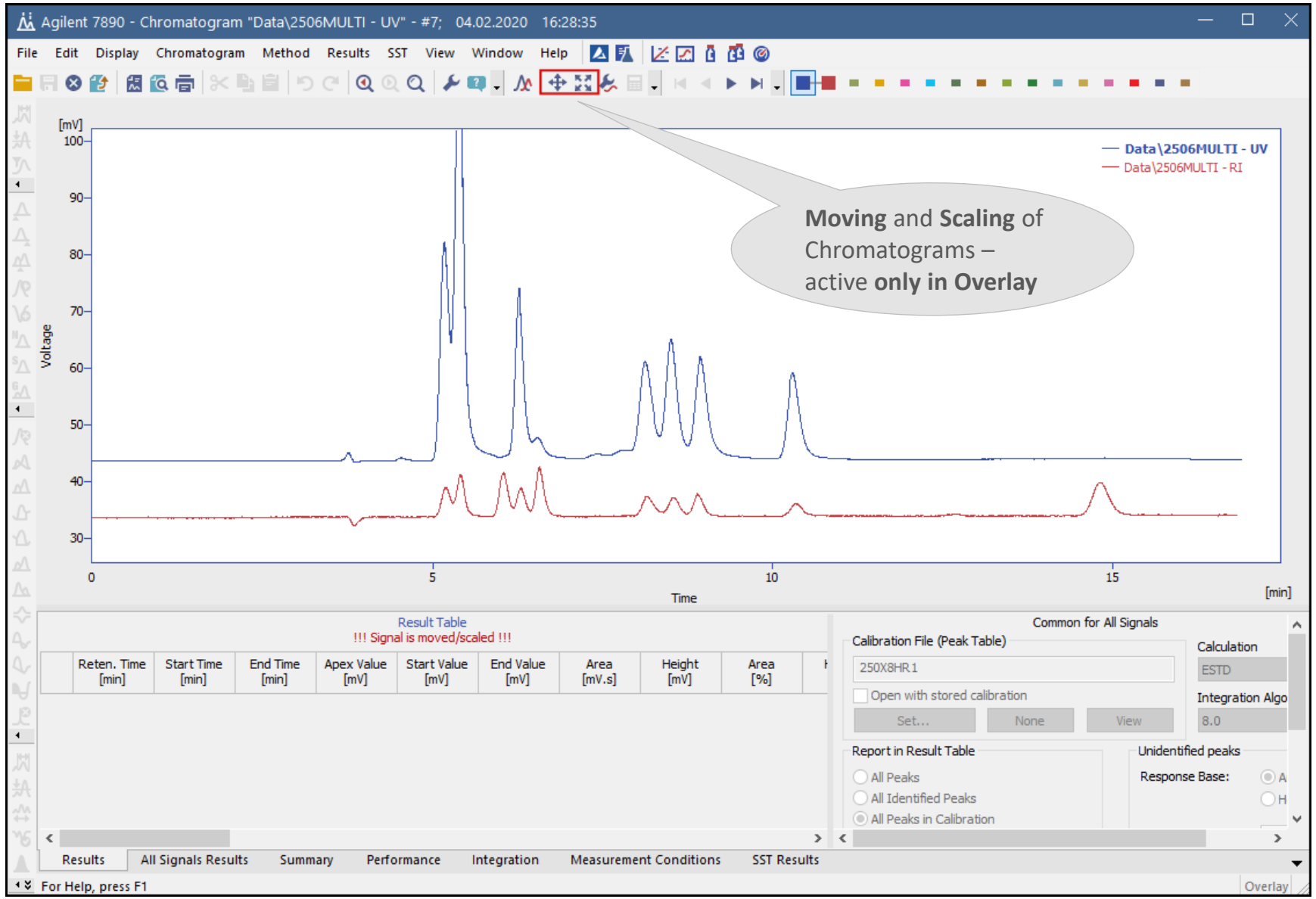


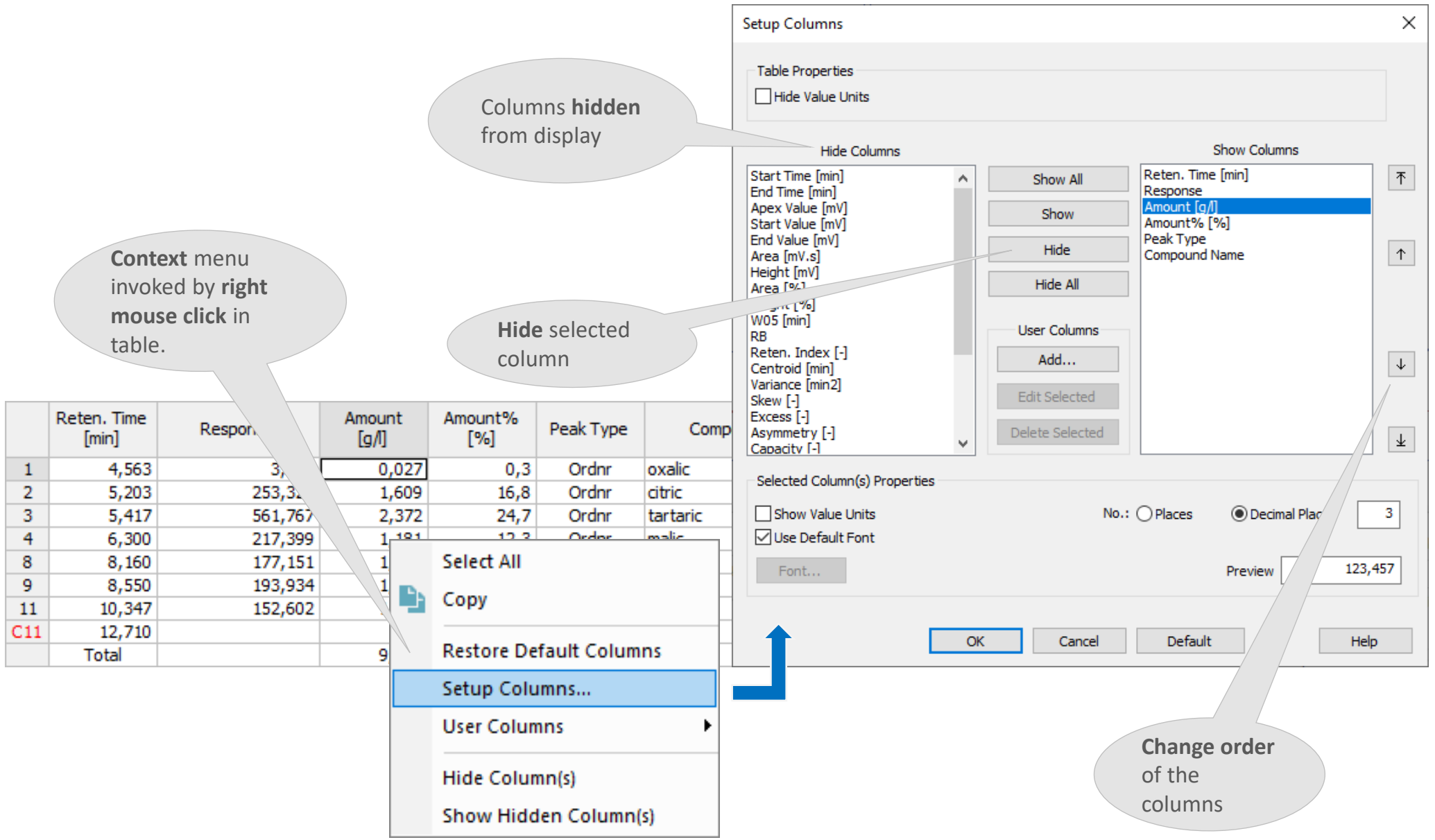
CHROMATOGRAM WINDOW → TEXT LABELS




Agilent 7890 - Chromatogram "Data\A-B - Signal 1" - #2; 01.04.2020 16:05:15
File Edit Display Chromatogram Method Results SST View Window Help
Mathematics
Mathematical operations with chromatograms. (Active only in Overlay mode.)
Math operations – active only in Overlay
Choose operands and operation to be performed
Data\A-B - Signal 1
[mV]
Voltage
Time
Result Table (Uncal - Data\A-B - Signal 1)
Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] | Compound Name
1 0,807 101,788 16,640 1,1 3,2 0,14
2 1,090 1036,582 48,263 11,6 9,2 0,33
3 1,707 815,404 76,563 9,1 14,7 0,13
4 2,207 519,629 58,484 5,8 11,2 0,16
5 2,427 1002,589 59,403 11,2 11,4 0,24
6 3,513 698,246 46,939 7,8 9,0 0,20
7 4,433 1390,697 82,494 15,5 15,8 0,24
8 5,447 723,757 34,879 8,1 6,7 0,30
9 6,233 695,782 30,504 7,8 5,8 0,31
10 7,287 257,871 13,277 2,9 2,5 0,30
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
Mathematical operations with chromatograms. (Active only in Overlay mode.)
Mathematical Operations
Operand A
The Whole Chromatogram
Data\Benzine1
Operation
Copy
Invert
Differentiate
A + B
A - B
Operand B
The Whole Chromatogram
Data\Solvent
Apply Method
Demo3
Save As Chromatogram
A-B
OK
Cancel
Help

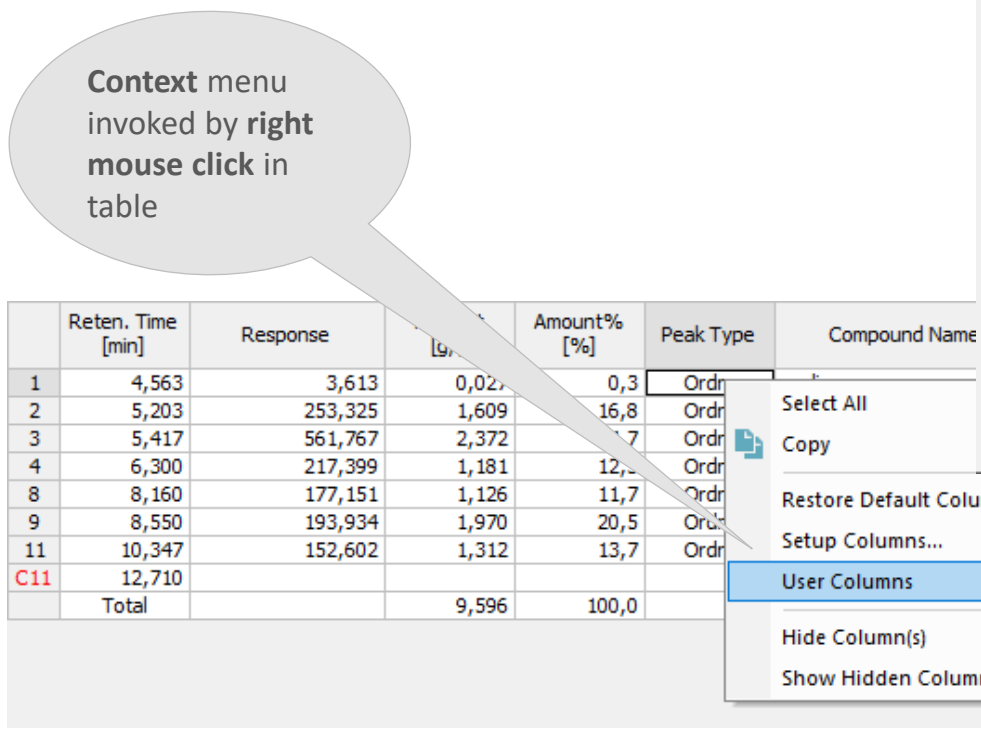
CHROMATOGRAM WINDOW → MOVE & SCALE

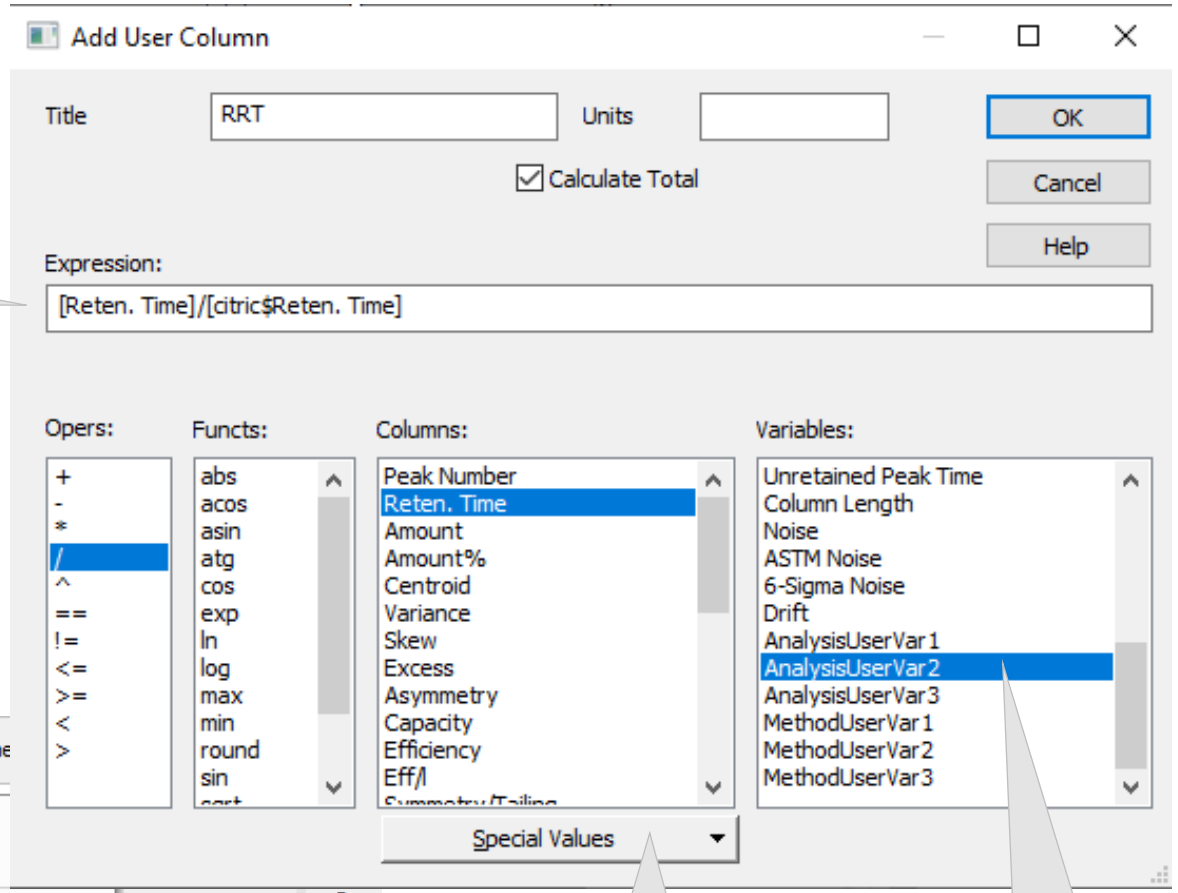



Columns **hidden** from display
Context menu invoked by **right mouse click** in table.
Hide selected column
Change order of the columns
Setup Columns
Table Properties
Hide Value Units
Hide Columns
Start Time [min]
End Time [min]
Apex Value [mV]
Start Value [mV]
End Value [mV]
Area [mV.s]
Height [mV]
W05 [min]
RB
Reten. Index [-]
Centroid [min]
Variance [min2]
Skew [-]
Excess [-]
Asymmetry [-]
Show All
Show
Hide
Hide All
User Columns
Add...
Edit Selected
Delete Selected
Show Columns
Reten. Time [min]
Response
Amount [g/l]
Amount% [%]
Peak Type
Compound Name
Selected Column(s) Properties
Show Value Units
Use Default Font
Font...
No.: Places
Decimal Plac
3
Preview
123,457
OK
Cancel
Default
Help
Reten. Time [min]
Amount [g/l]
Amount% [%]
Peak Type
1 4,563 0,027 0,3 Ordnr oxalic
2 5,203 1,609 16,8 Ordnr citric
3 5,417 2,372 24,7 Ordnr tartaric
4 6,300
8 8,160
9 8,550
11 10,347 152,602
C11 12,710
Total
Select All
Copy
Restore Default Columns
Setup Columns...
User Columns
Hide Column(s)
Show Hidden Column(s)

Custom calculations using **User columns**

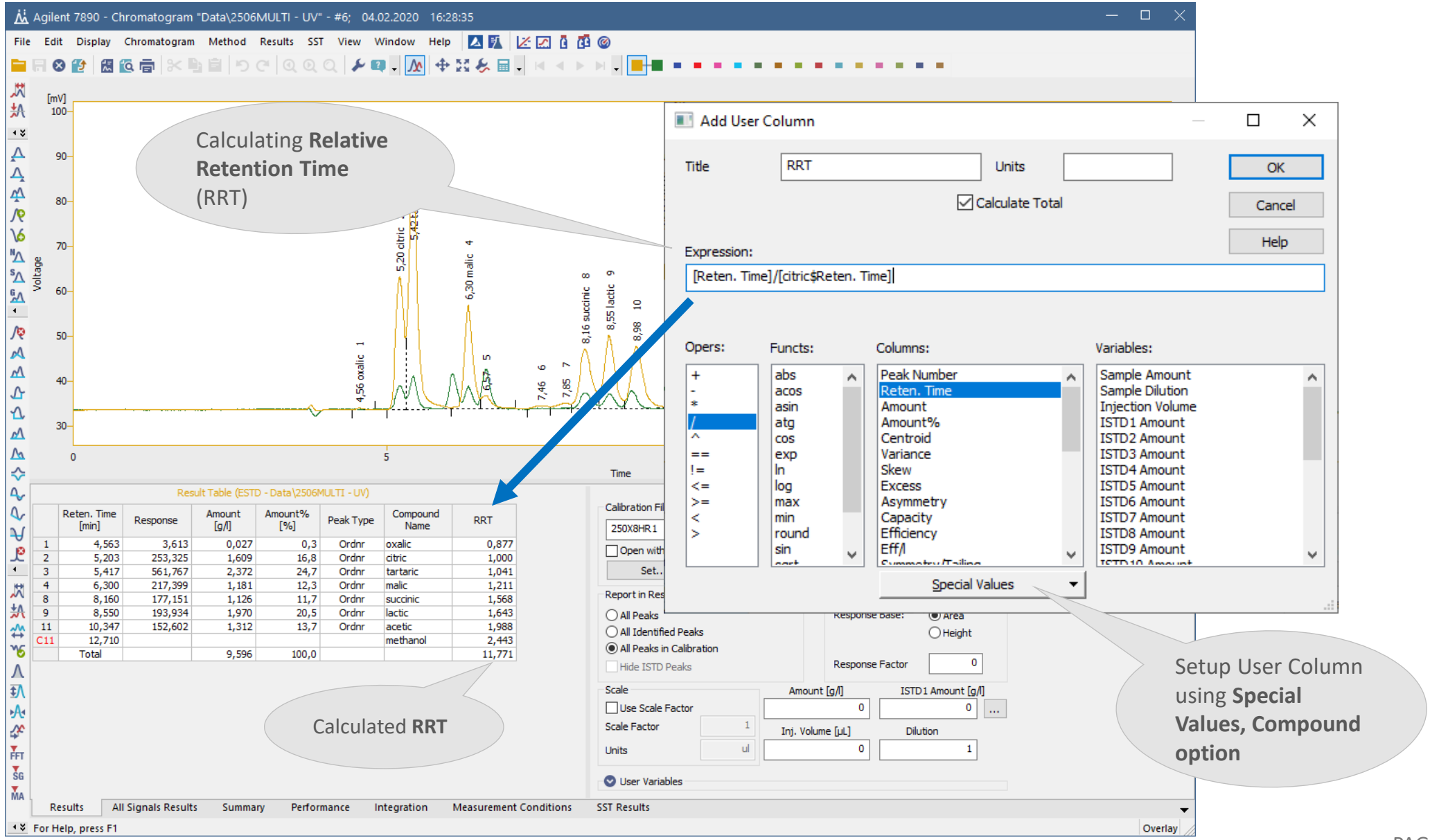
Context menu invoked by **right mouse click** in table

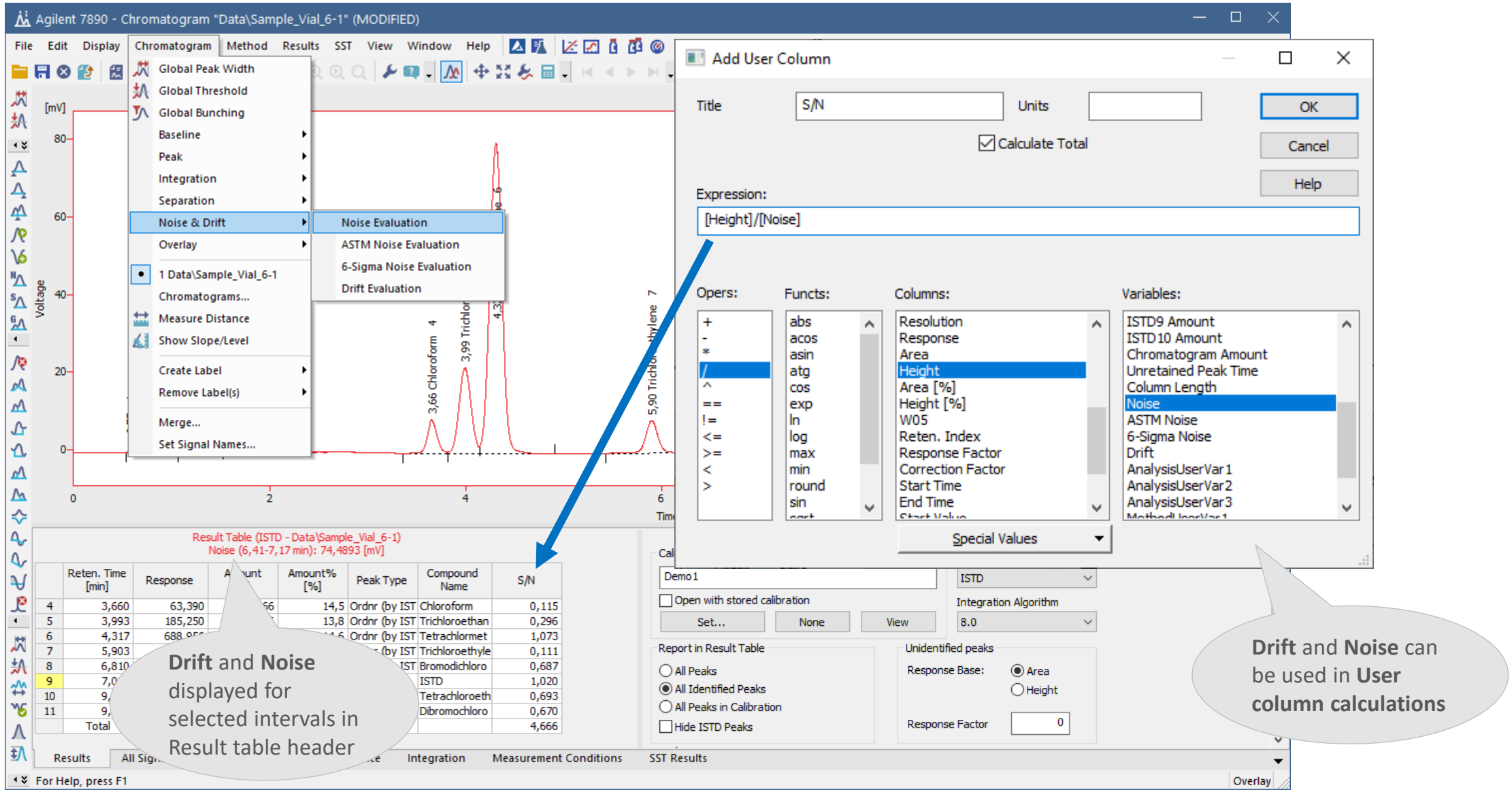




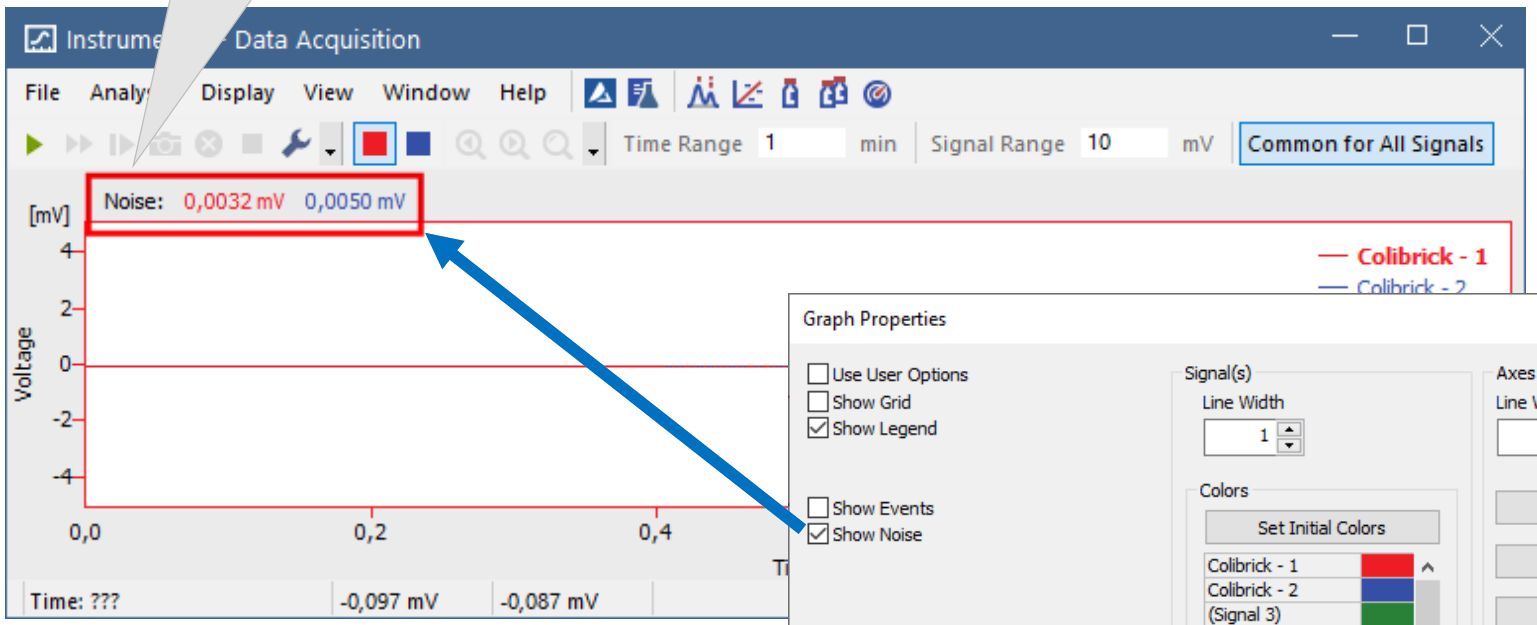
Special values for advanced features

Large variability using **user** and **method** variables

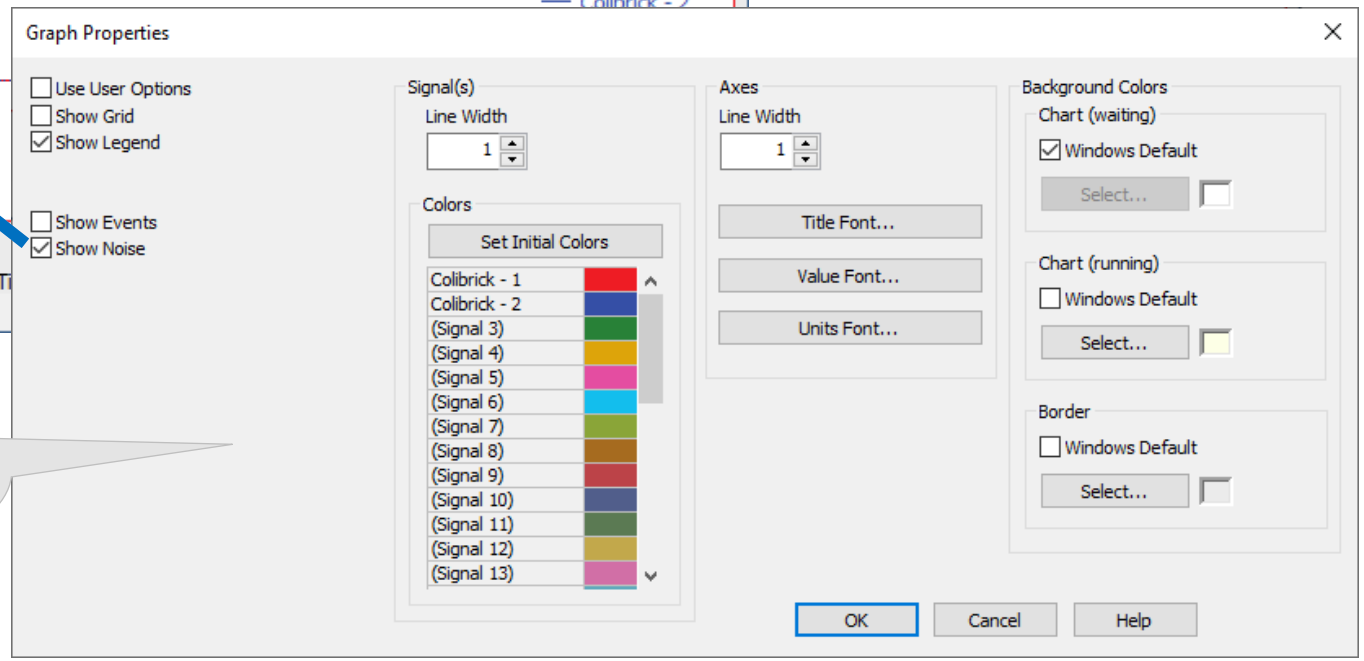

Agilent 7890 - Chromatogram "Data\2506MULTI - UV" - #6; 04.02.2020 16:28:35
File Edit Display Chromatogram Method Results SST View Window Help
Calculating **Relative Retention Time** (RRT)
Add User Column
Title
RRT
Units
OK
Cancel
Help
Calculate Total
Expression:
[Reten. Time]/[citric$Reten. Time]
Opers:
Functs:
Columns:
Variables:
Peak Number
Reten. Time
Amount
Amount%
Centroid
Variance
Skew
Excess
Asymmetry
Capacity
Efficiency
Eff/l
Sample Amount
Sample Dilution
Injection Volume
ISTD1 Amount
ISTD2 Amount
ISTD3 Amount
ISTD4 Amount
ISTD5 Amount
ISTD6 Amount
ISTD7 Amount
ISTD8 Amount
ISTD9 Amount
Special Values
Result Table (ESTD - Data\2506MULTI - UV)
Reten. Time [min] | Response | Amount [g/l] | Amount% [%] | Peak Type | Compound Name | RRT
1 | 4,563 | 3,613 | 0,027 | 0,3 | Ordnr | oxalic | 0,877
2 | 5,203 | 253,325 | 1,609 | 16,8 | Ordnr | citric | 1,000
3 | 5,417 | 561,767 | 2,372 | 24,7 | Ordnr | tartaric | 1,041
4 | 6,300 | 217,399 | 1,181 | 12,3 | Ordnr | malic | 1,211
8 | 8,160 | 177,151 | 1,126 | 11,7 | Ordnr | succinic | 1,568
9 | 8,550 | 193,934 | 1,970 | 20,5 | Ordnr | lactic | 1,643
11 | 10,347 | 152,602 | 1,312 | 13,7 | Ordnr | acetic | 1,988
C11 | 12,710 | | | | | methanol | 2,443
Total | | 9,596 | 100,0 | | | 11,771
Calculated **RRT**
Setup User Column using **Special Values, Compound option**
Results
All Signals Results
Summary
Performance
Integration
Measurement Conditions
SST Results
For Help, press F1
Overlay


Agilent 7890 - Chromatogram "Data\Sample_Vial_6-1" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
Global Peak Width
Global Threshold
Global Bunching
Baseline
Peak
Integration
Separation
Noise & Drift
Overlay
1 Data\Sample_Vial_6-1
Chromatograms...
Measure Distance
Show Slope/Level
Create Label
Remove Label(s)
Merge...
Set Signal Names...
Noise Evaluation
ASTM Noise Evaluation
6-Sigma Noise Evaluation
Drift Evaluation
Add User Column
Title
S/N
Units
OK
Cancel
Help
Calculate Total
Expression:
[Height]/[Noise]
Opers:
Functs:
Columns:
Variables:
Resolution
Response
Area
Height
Area [%]
Height [%]
W05
Reten. Index
Response Factor
Correction Factor
Start Time
End Time
ISTD9 Amount
ISTD10 Amount
Chromatogram Amount
Unretained Peak Time
Column Length
Noise
ASTM Noise
6-Sigma Noise
Drift
AnalysisUserVar1
AnalysisUserVar2
AnalysisUserVar3
Special Values
Result Table (ISTD - Data\Sample_Vial_6-1)
Noise (6,41-7,17 min): 74,4893 [mV]
Reten. Time [min]
Response
Amount%
Peak Type
Compound Name
S/N
Chloroform
Trichloroethan
Tetrachlormet
Trichloroethyle
Bromodichloro
ISTD
Tetrachloroeth
Dibromochloro
Demo1
Open with stored calibration
Set...
None
View
ISTD
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
Drift and Noise displayed for selected intervals in Result table header
Drift and Noise can be used in User column calculations
Results
Integration
Measurement Conditions
SST Results
For Help, press F1
Overlay

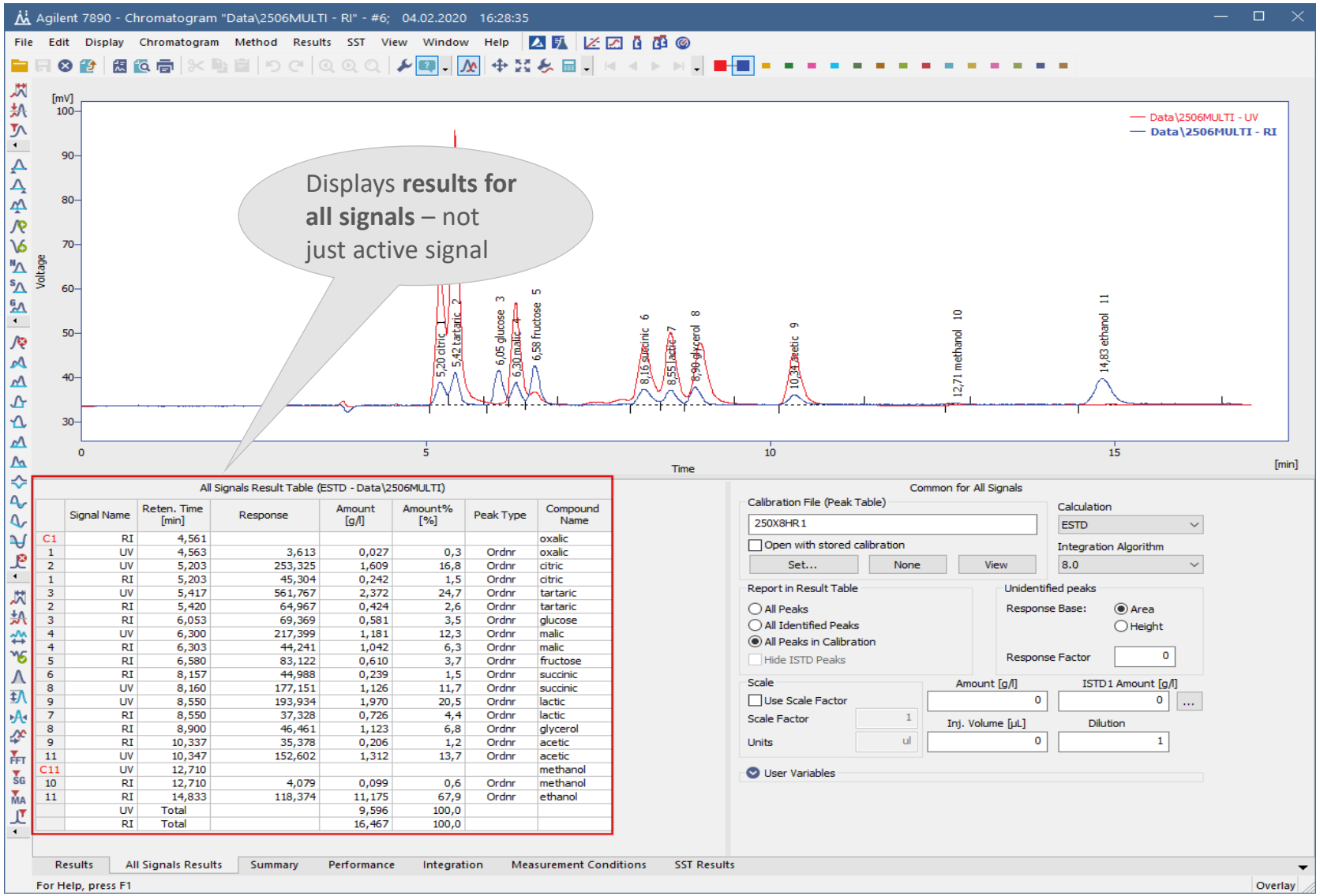
Actual **noise monitoring** in the Data Acquisition window



Invoked by **right mouse click in graph area**



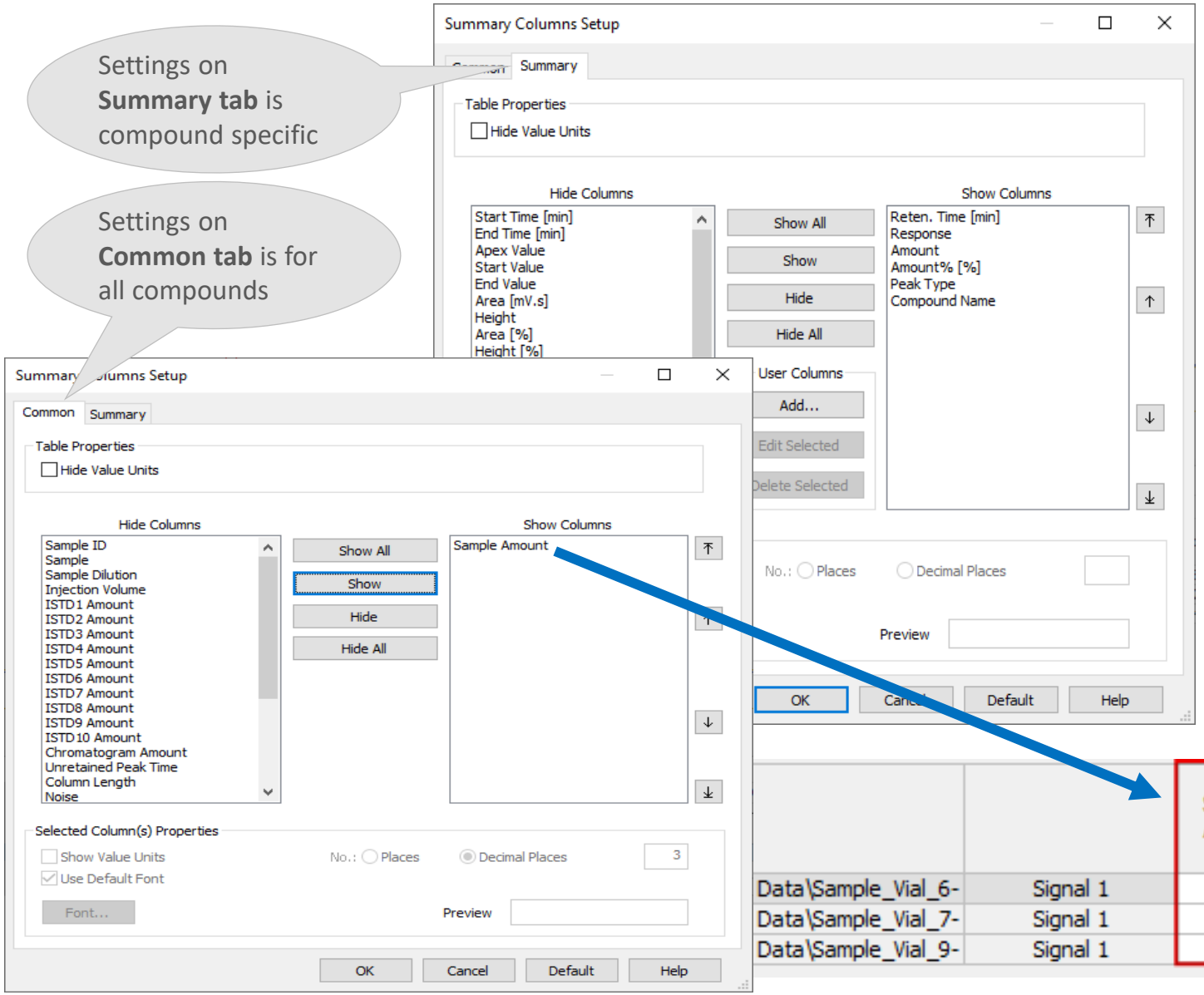
CHROMATOGRAM WINDOW → ALL SIGNALS RESULT TABLE



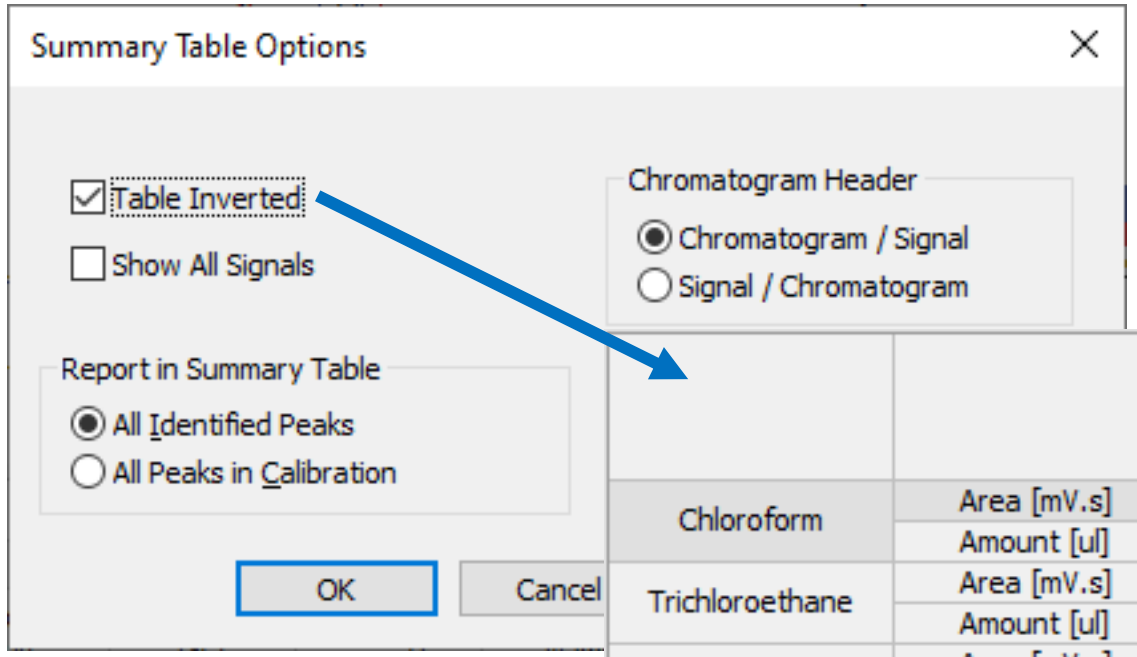
	Signal Name	Reten. Time [min]	Response	Amount [g/l]	Amount% [%]	Peak Type	Compound Name
C1	RI	4,561					oxalic
1	UV	4,563	3,613	0,027	0,3	Ordnr	oxalic
2	UV	5,203	253,325	1,609	16,8	Ordnr	citric
1	RI	5,203	45,304	0,242	1,5	Ordnr	citric
3	UV	5,417	561,767	2,372	24,7	Ordnr	tartaric
2	RI	5,420	64,967	0,424	2,6	Ordnr	tartaric
3	RI	6,053	69,369	0,581	3,5	Ordnr	glucose
4	UV	6,300	217,399	1,181	12,3	Ordnr	malic
4	RI	6,303	44,241	1,042	6,3	Ordnr	malic
5	RI	6,580	83,122	0,610	3,7	Ordnr	fructose
6	RI	8,157	44,988	0,239	1,5	Ordnr	succinic
8	UV	8,160	177,151	1,126	11,7	Ordnr	succinic
9	UV	8,550	193,934	1,970	20,5	Ordnr	lactic
7	RI	8,550	37,328	0,726	4,4	Ordnr	lactic
8	RI	8,900	46,461	1,123	6,8	Ordnr	glycerol
9	RI	10,337	35,378	0,206	1,2	Ordnr	acetic
11	UV	10,347	152,602	1,312	13,7	Ordnr	acetic
C11	UV	12,710					methanol
10	RI	12,710	4,079	0,099	0,6	Ordnr	methanol
11	RI	14,833	118,374	11,175	67,9	Ordnr	ethanol
	UV	Total		9,596	100,0		
	RI	Total		16,467	100,0		

Settings on **Summary tab** is compound specific

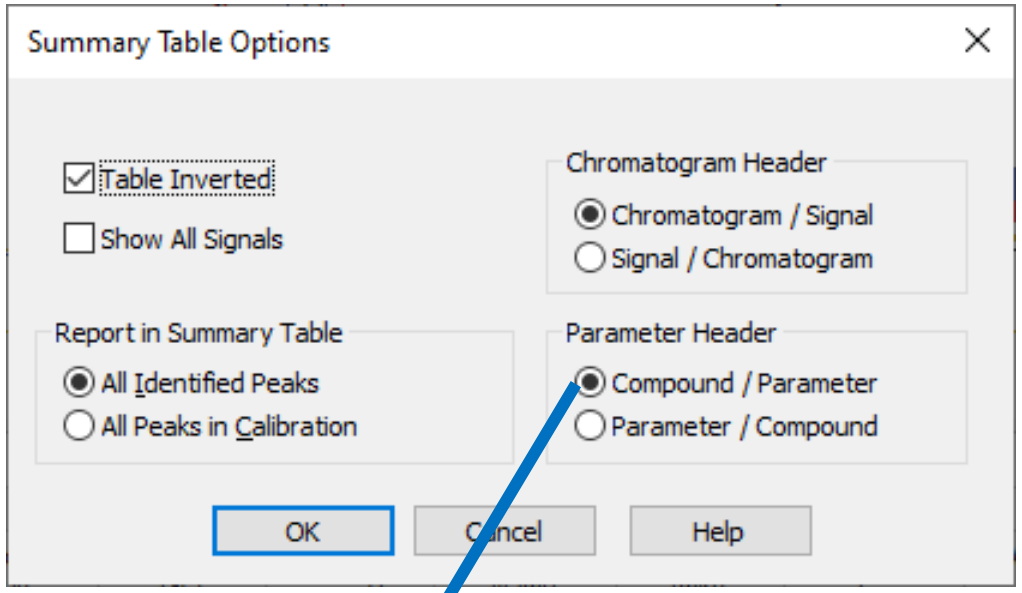
Settings on **Common tab** is for all compounds



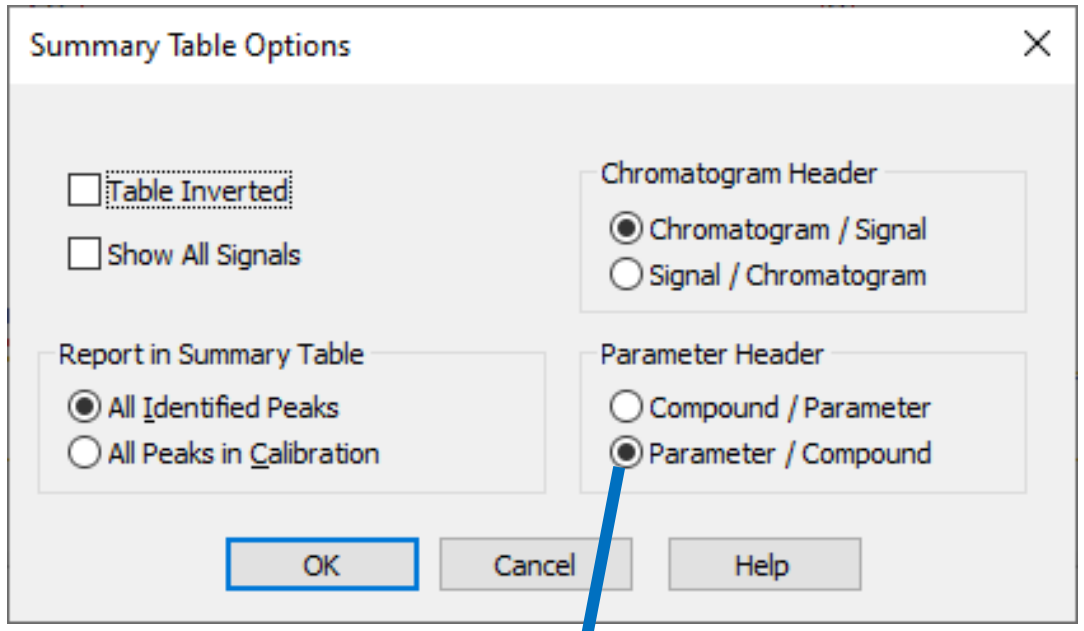
		Sample Amount	Reten. Time [min]	Response
Data\Sample_Vial_6-	Signal 1	0,000	3,660	63,390
Data\Sample_Vial_7-	Signal 1	0,000	3,680	272,107
Data\Sample_Vial_9-	Signal 1	0,000	3,647	140,237



		Data\Sample_Vial_6-	Data\Sample_Vial_7-	Data\Sample_Vial_9-
		Signal 1	Signal 1	Signal 1
Chloroform	Area [mV.s]	63,390	272,107	140,237
	Amount [ul]	1,266 ul	4,876 ul	2,842 ul
Trichloroethane	Area [mV.s]	185,250	806,068	419,318
	Amount [ul]	1,206 ul	4,709 ul	2,770 ul
Tetrachlormethane	Area [mV.s]	688,956	2725,112	1541,388
	Amount [ul]	1,277 ul	4,533 ul	2,899 ul
Trichloroethylene	Area [mV.s]	69,023	306,636	156,032
	Amount [ul]	1,248 ul	4,975 ul	2,863 ul
Bromodichloroethane	Area [mV.s]	378,298	1634,130	870,847
	Amount [ul]	1,209 ul	4,685 ul	2,823 ul
ISTD	Area [mV.s]	639,259	712,393	629,957
	Amount [ul]	ISTD	ISTD	ISTD

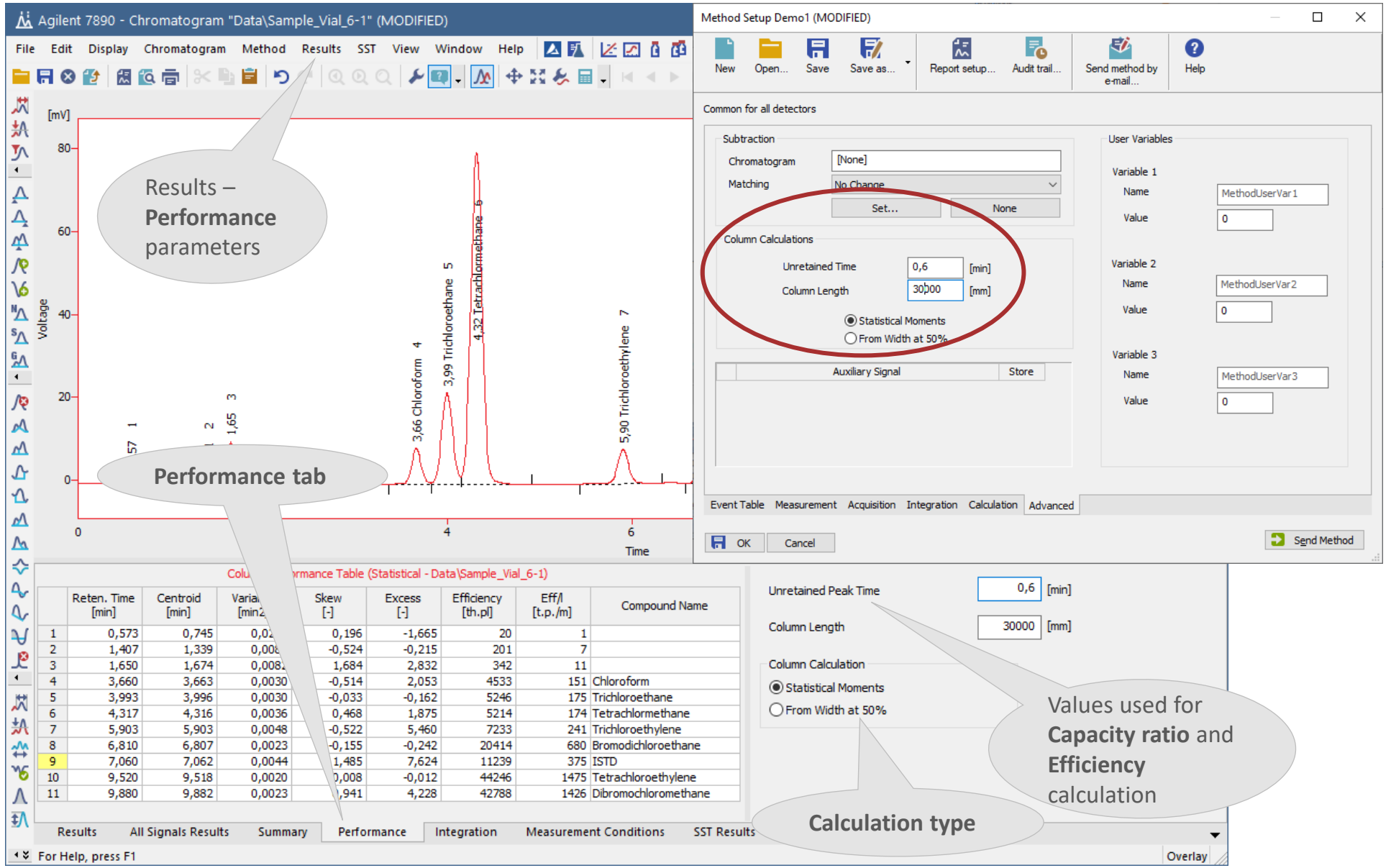


		Sample Amount	Chloroform		Trichloroethane		Tetrachlormethane	
			Area [mV.s]	Amount [ul]	Area [mV.s]	Amount [ul]	Area [mV.s]	Amount [ul]
Data\Sample_Vial_6-	Signal 1	0,000	63,390	1,266 ul	185,250	1,206 ul	688,956	1,277 ul
Data\Sample_Vial_7-	Signal 1	0,000	272,107	4,876 ul	806,068	4,709 ul	2725,112	4,533 ul
Data\Sample_Vial_9-	Signal 1	0,000	140,237	2,842 ul	419,318	2,770 ul	1541,388	2,899 ul

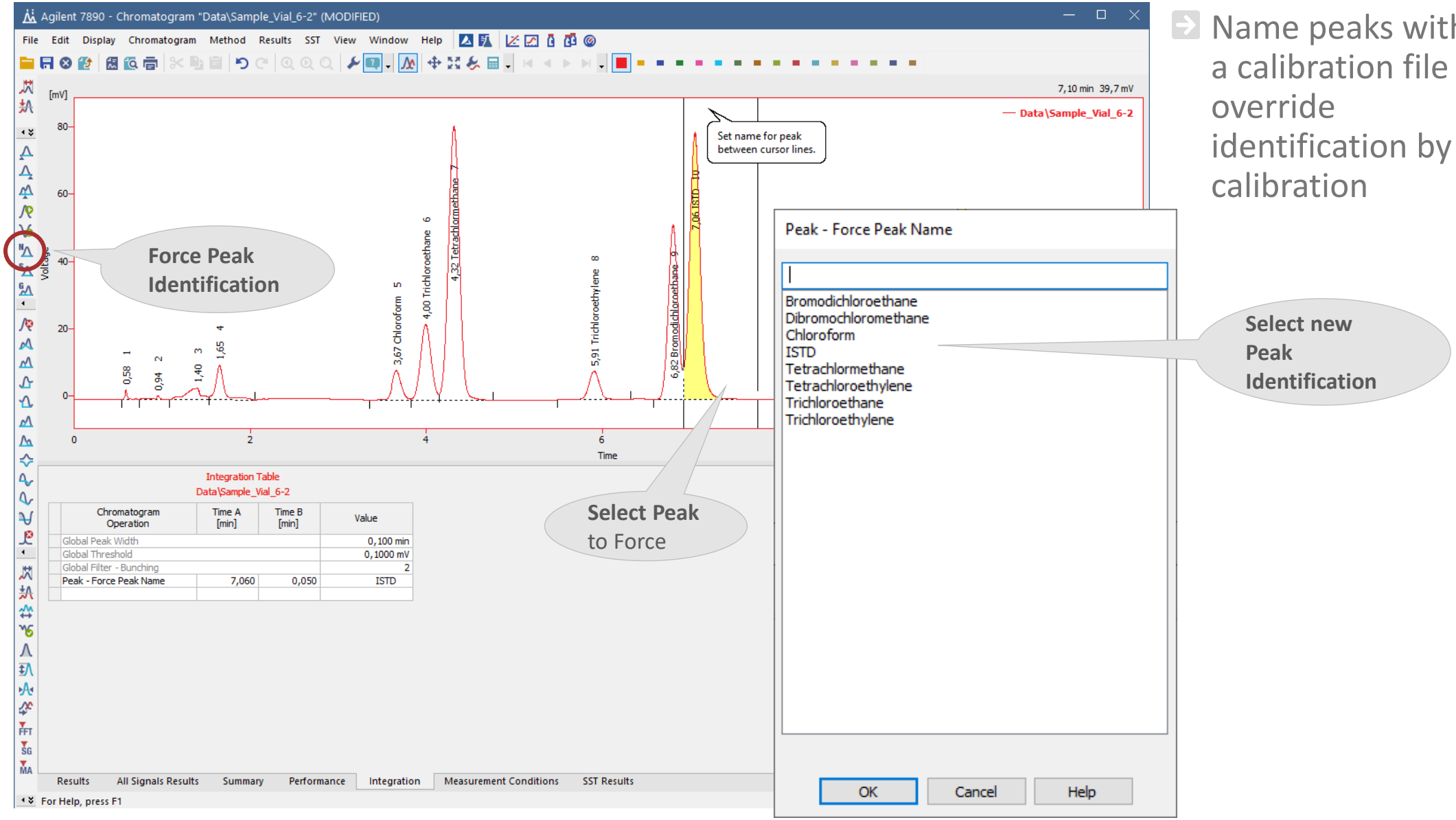


		Sample Amount	Area [mV.s]				
			Chloroform	Trichloroethane	Tetrachlormethane	Trichloroethylene	Bromodichloroethane
Data\Sample_Vial_6-	Signal 1	0,000	63,390	185,250	688,956	69,023	378,298
Data\Sample_Vial_7-	Signal 1	0,000	272,107	806,068	2725,112	306,636	1634,130
Data\Sample_Vial_9-	Signal 1	0,000	140,237	419,318	1541,388	156,032	870,847

CHROMATOGRAM WINDOW → PERFORMANCE TAB

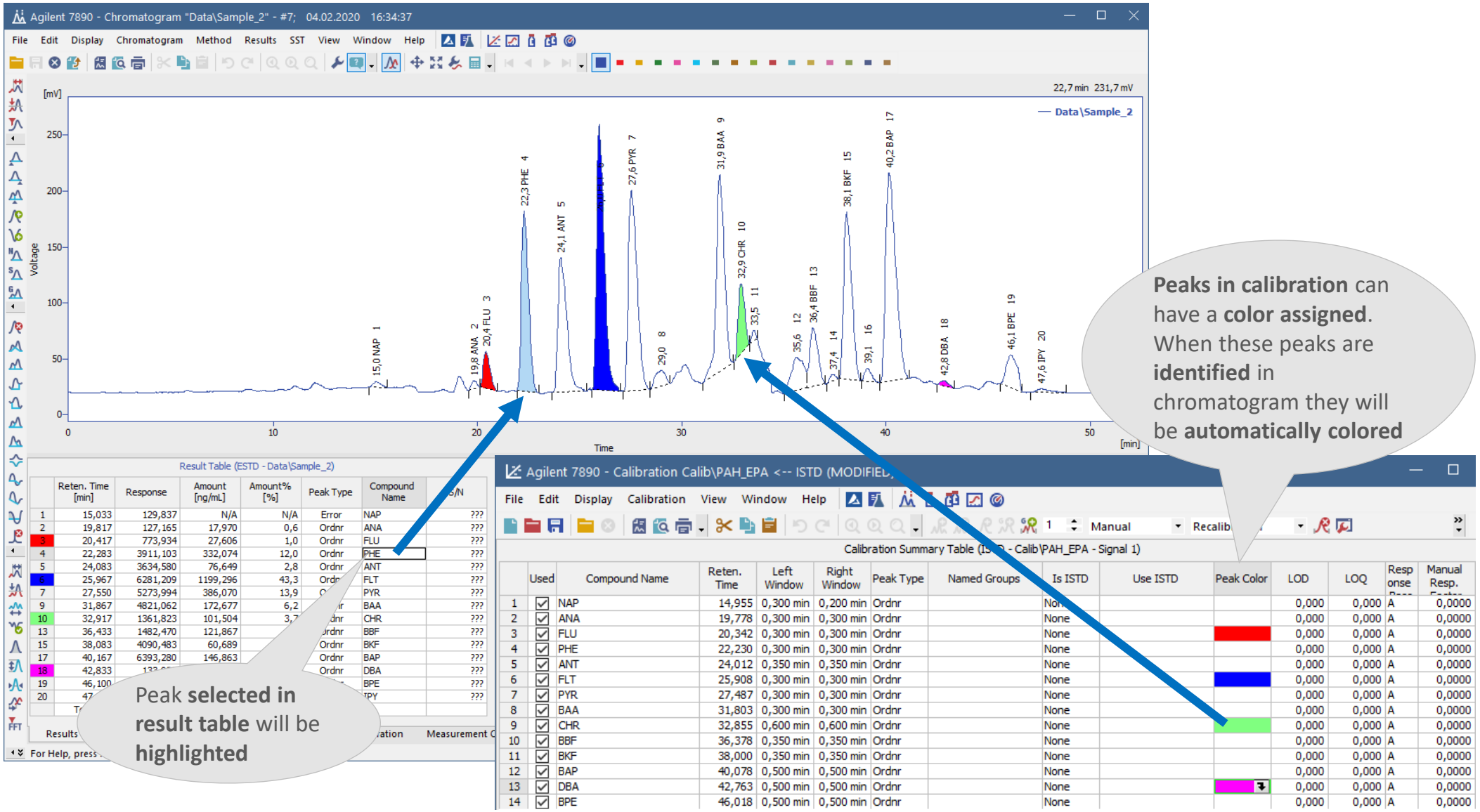


CHROMATOGRAM WINDOW → FORCE PEAK NAME FUNCTION

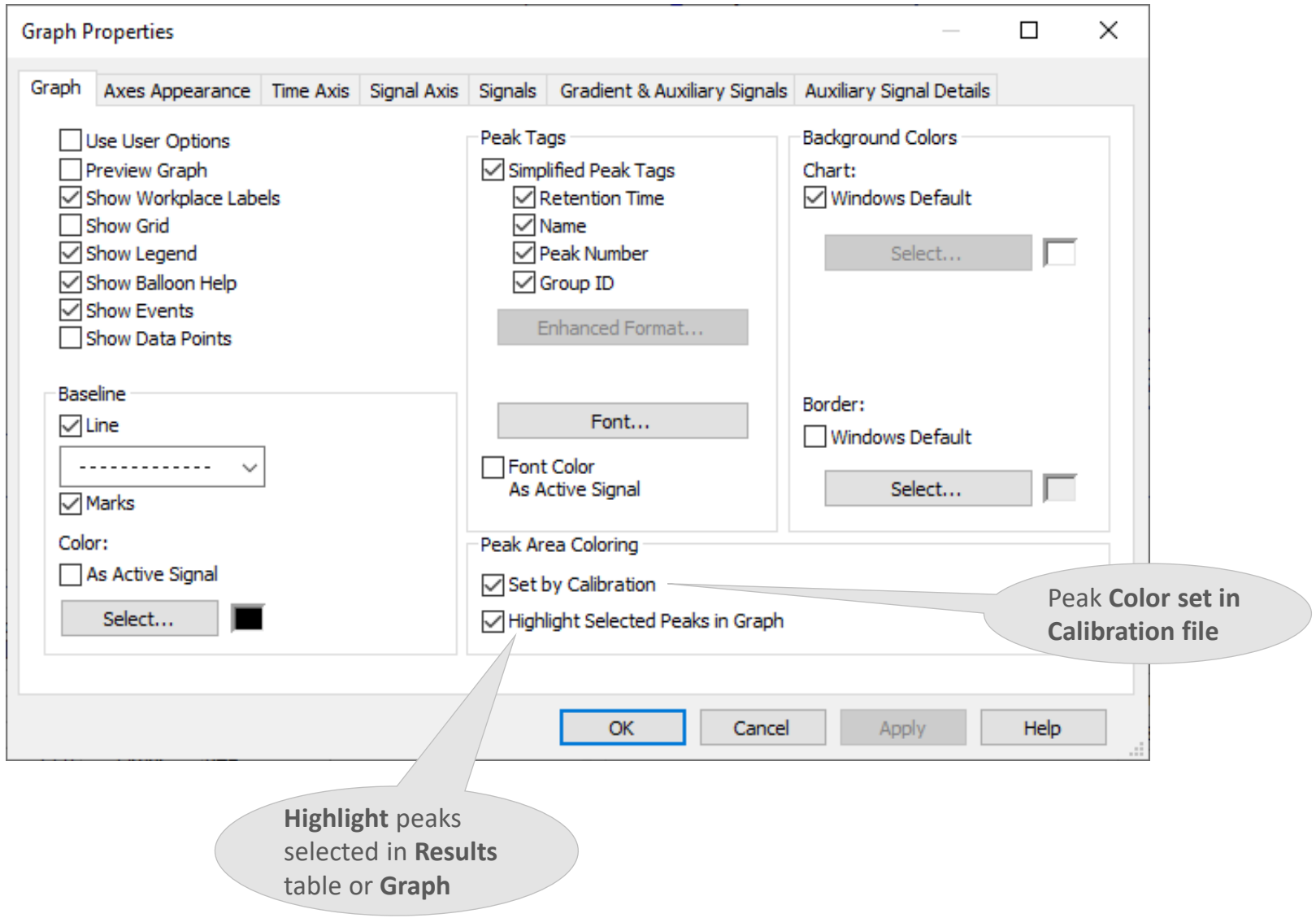


- Name peaks without a calibration file or override identification by calibration

CHROMATOGRAM WINDOW → PEAK COLORING

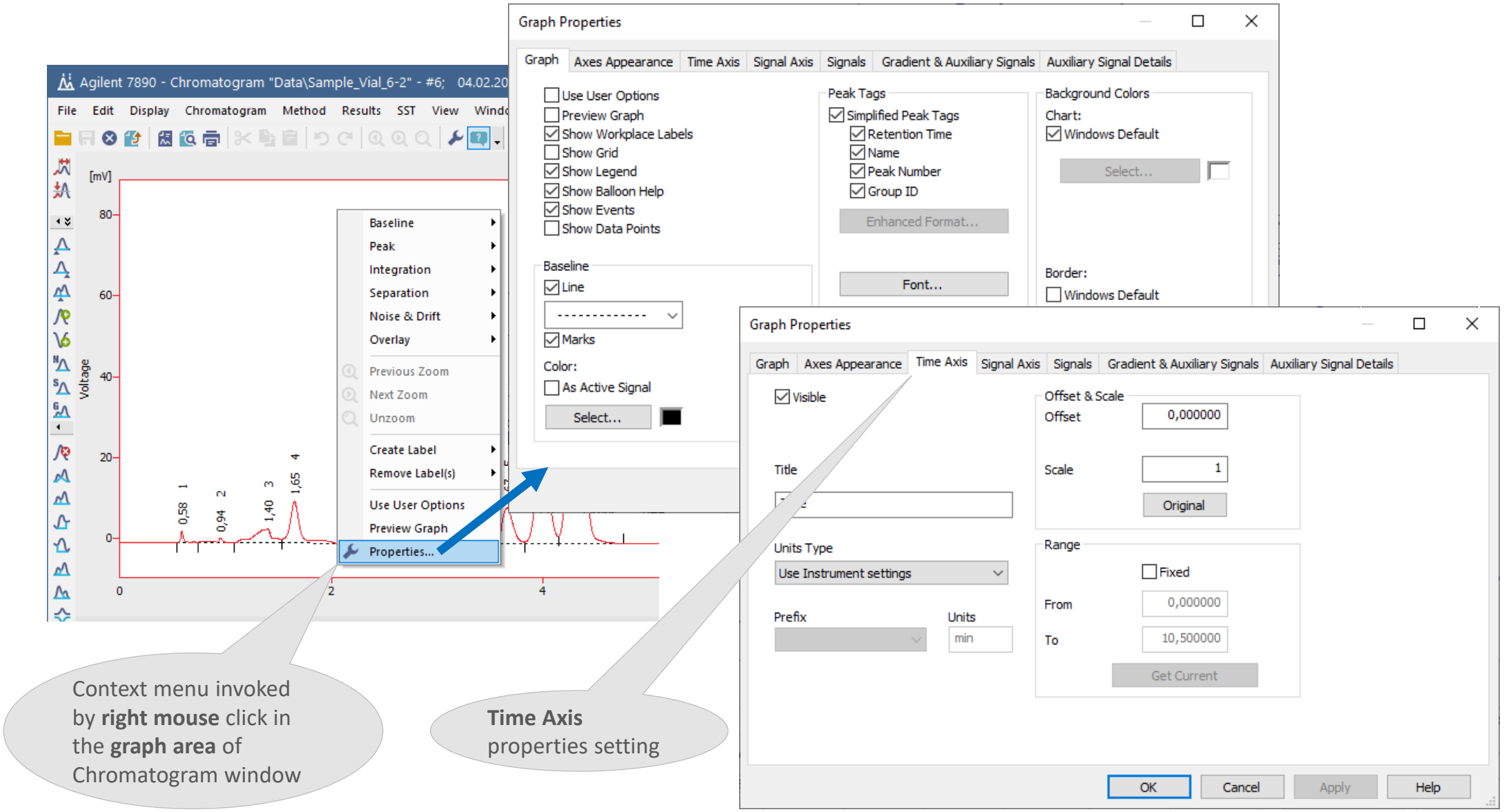


	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response	Manual Resp.
1	☑	NAP	14,955	0,300 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000
2	☑	ANA	19,778	0,300 min	0,300 min	Ordnr		None			0,000	0,000	A	0,0000
3	☑	FLU	20,342	0,300 min	0,300 min	Ordnr		None			0,000	0,000	A	0,0000
4	☑	PHE	22,230	0,300 min	0,300 min	Ordnr		None			0,000	0,000	A	0,0000
5	☑	ANT	24,012	0,350 min	0,350 min	Ordnr		None			0,000	0,000	A	0,0000
6	☑	FLT	25,908	0,300 min	0,300 min	Ordnr		None			0,000	0,000	A	0,0000
7	☑	PYR	27,487	0,300 min	0,300 min	Ordnr		None			0,000	0,000	A	0,0000
8	☑	BAA	31,803	0,300 min	0,300 min	Ordnr		None			0,000	0,000	A	0,0000
9	☑	CHR	32,855	0,600 min	0,600 min	Ordnr		None			0,000	0,000	A	0,0000
10	☑	BBF	36,378	0,350 min	0,350 min	Ordnr		None			0,000	0,000	A	0,0000
11	☑	BKF	38,000	0,350 min	0,350 min	Ordnr		None			0,000	0,000	A	0,0000
12	☑	BAP	40,078	0,500 min	0,500 min	Ordnr		None			0,000	0,000	A	0,0000
13	☑	DBA	42,763	0,500 min	0,500 min	Ordnr		None			0,000	0,000	A	0,0000
14	☑	BPE	46,018	0,500 min	0,500 min	Ordnr		None			0,000	0,000	A	0,0000



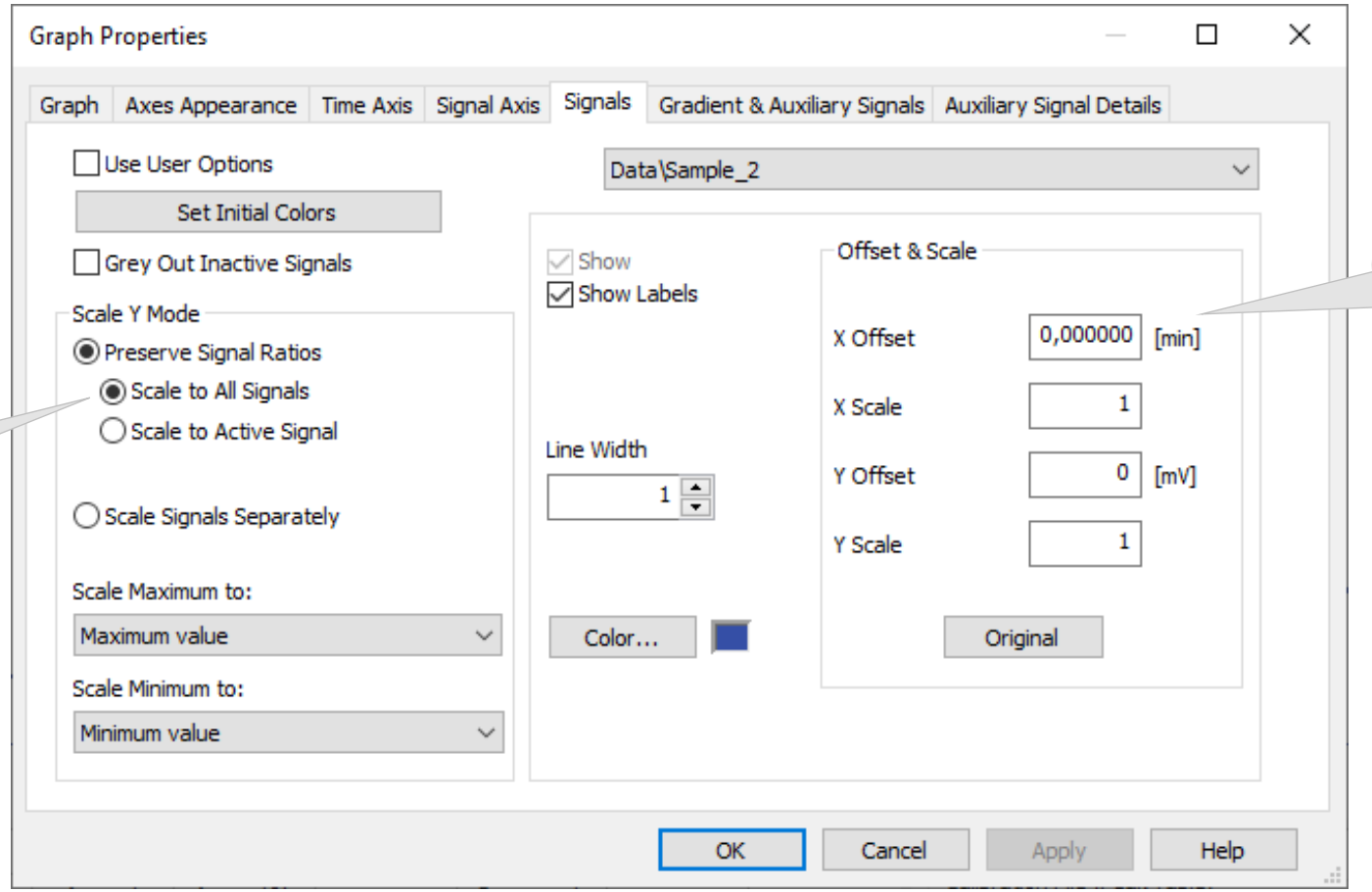
Peak **Color set in Calibration file**

Highlight peaks selected in **Results** table or **Graph**



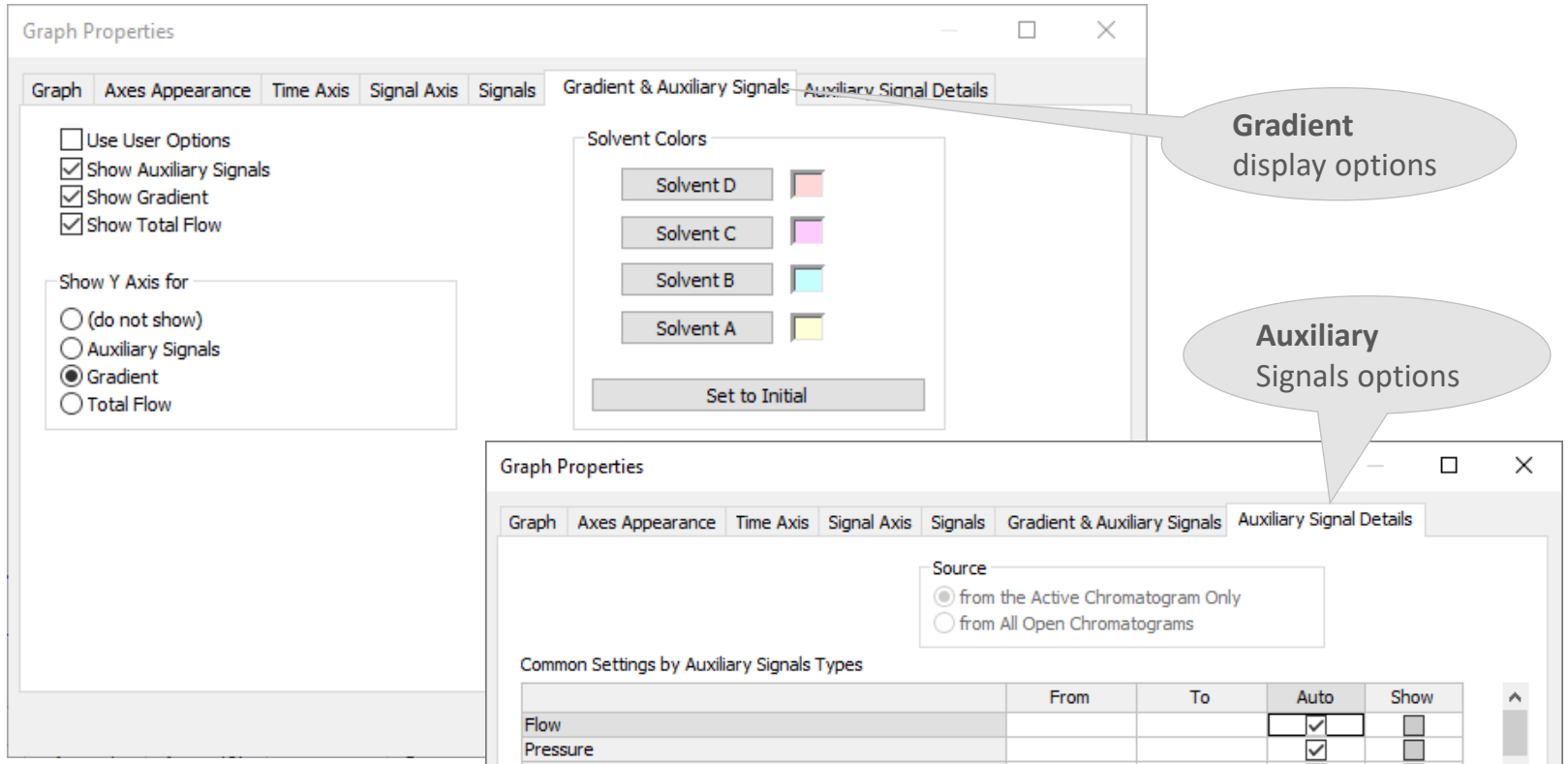
Context menu invoked by **right mouse** click in the **graph area** of Chromatogram window

Time Axis properties setting

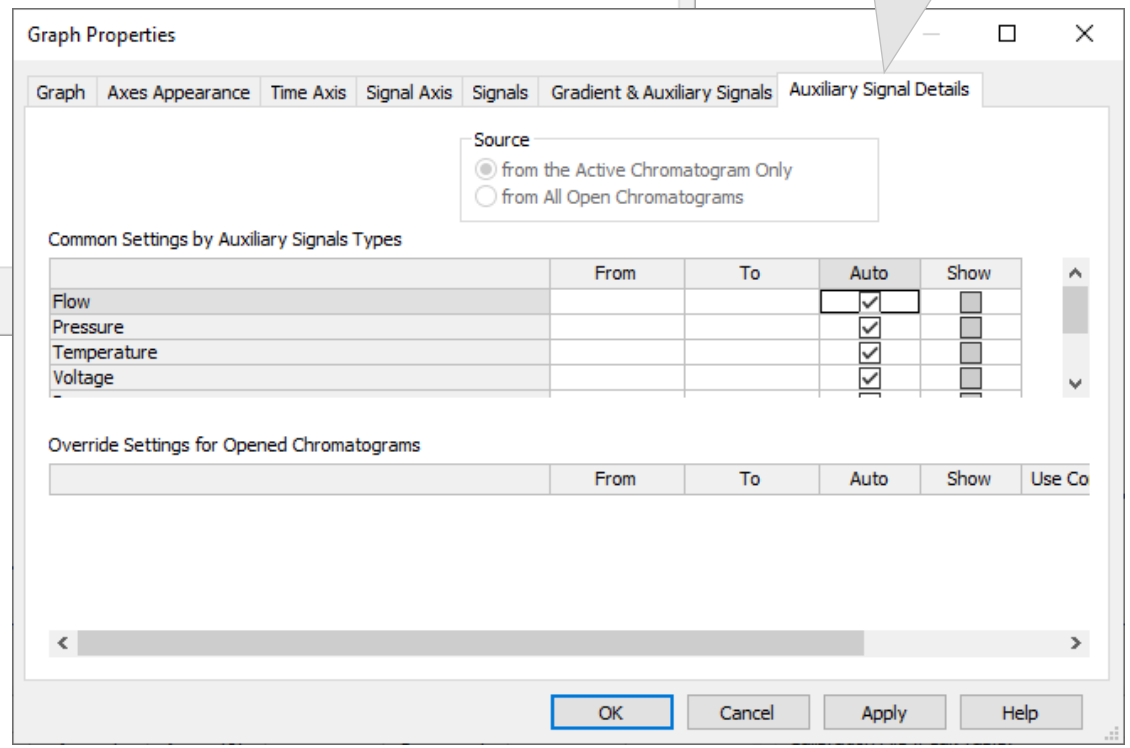


Signal **scaling**

Individual Signal settings **Scale** and **Move**



Gradient
display options

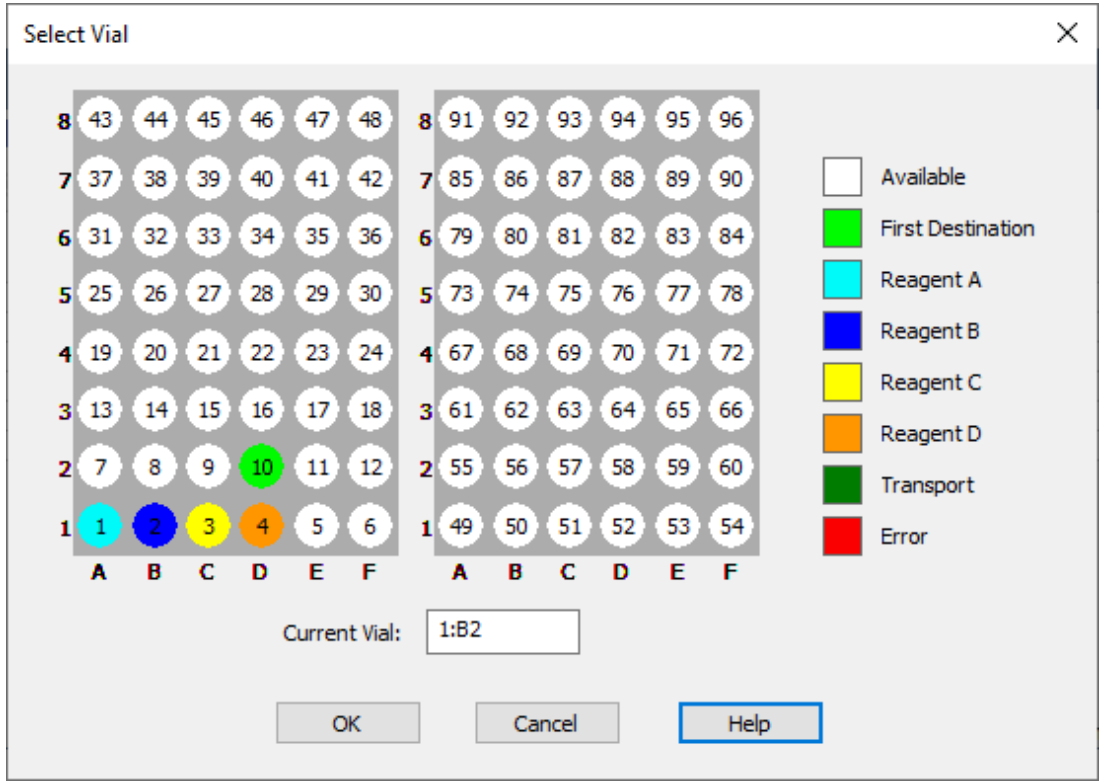


Auxiliary
Signals options

Agenda

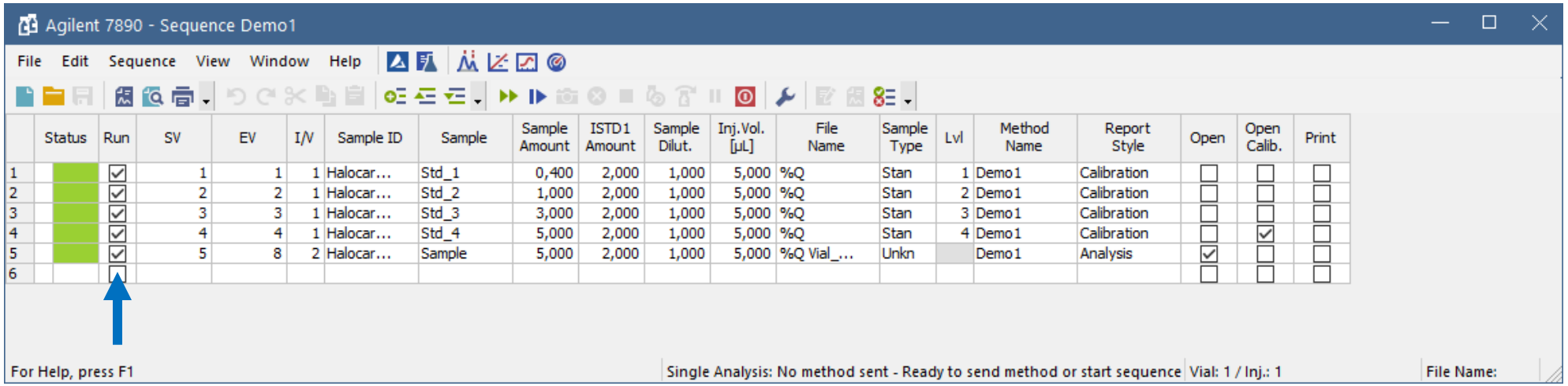
- Instrument window
- Chromatogram window
  - Overlay, 3D View and Labels
  - Setup columns
  - User columns
  - Noise and Drift
  - Performance tab
  - Force peak function
  - Peak coloring
  - Graph properties
- Sequence table
  - Overview
  - Description of sequence window
  - Basic functions
  - Sequence mode
  - Options
  - Import
  - Fill Series function

- Defines a **series of samples to be measured**
- Essential for working with **autosamplers**
- For controlled autosamplers the **Vial number** and **Injection volume** are loaded from this table
- **Graphical** interface



- Allows **modifications** during a run for **not yet processed samples**

- Simply **add samples** by filling any field in the **last empty row**
- Other fields will be **copied from previous row**
- Several samples can be added by **copying from a table**
- Allows the **import** of sample data from text files
- Allows **reprocessing of last measured** sample set



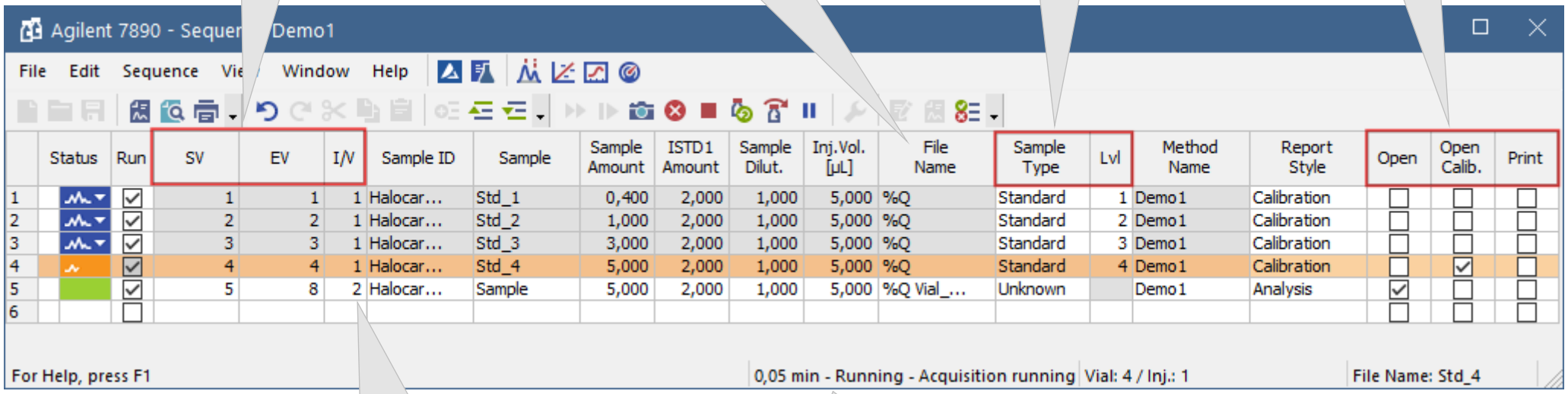
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1		☑	1	1	1	Halocar...	Std_1	0,400	2,000	1,000	5,000	%Q	Stan	1	Demo1	Calibration	☐	☐	☐
2		☑	2	2	1	Halocar...	Std_2	1,000	2,000	1,000	5,000	%Q	Stan	2	Demo1	Calibration	☐	☐	☐
3		☑	3	3	1	Halocar...	Std_3	3,000	2,000	1,000	5,000	%Q	Stan	3	Demo1	Calibration	☐	☐	☐
4		☑	4	4	1	Halocar...	Std_4	5,000	2,000	1,000	5,000	%Q	Stan	4	Demo1	Calibration	☐	☑	☐
5		☑	5	8	2	Halocar...	Sample	5,000	2,000	1,000	5,000	%Q Vial_...	Unkn		Demo1	Analysis	☑	☐	☐
6		☐															☐	☐	☐

Start, End vial and Injections number.

File name, automatic %variables for SV, EV, IV

Automatic **recalibration** from sequence

Individual **Post-Run settings** for each row

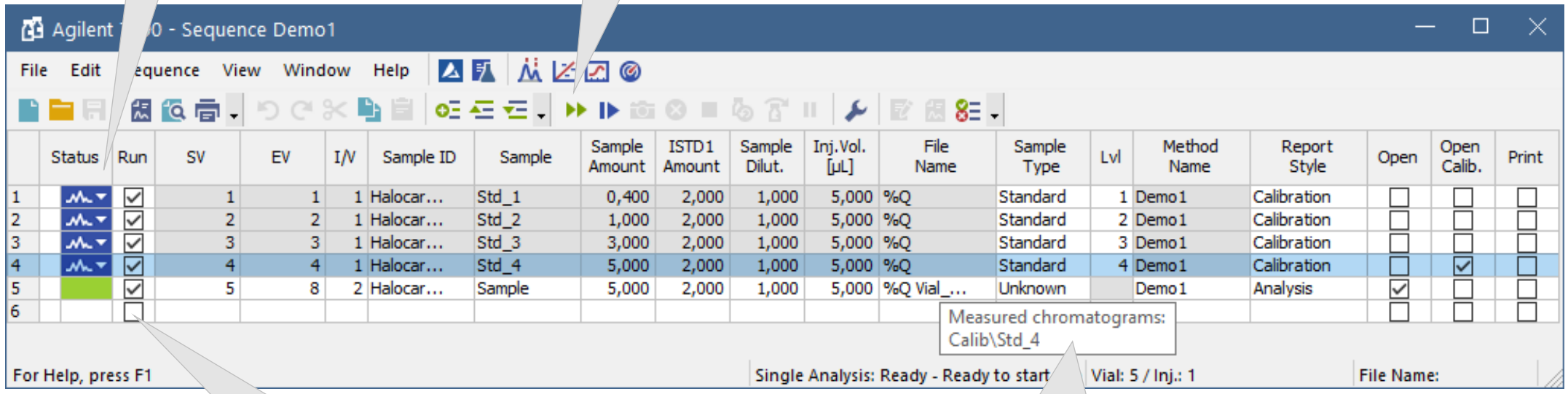


Several vials and/or injections defined on single row

Displays **the state of the sequence** – runtime etc.

Row status indicator

Run sequence starts a sequence (resets the status)



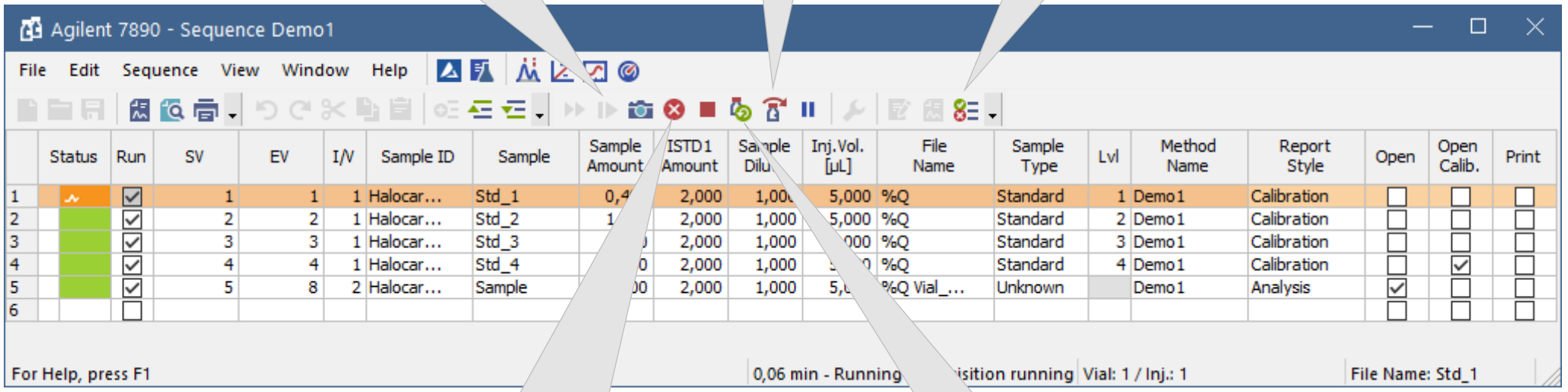
Use row, **add new rows during** sequence run

Tooltip with actual file name

Resume sequence continues from last injection

Skip vial

Check Sequence



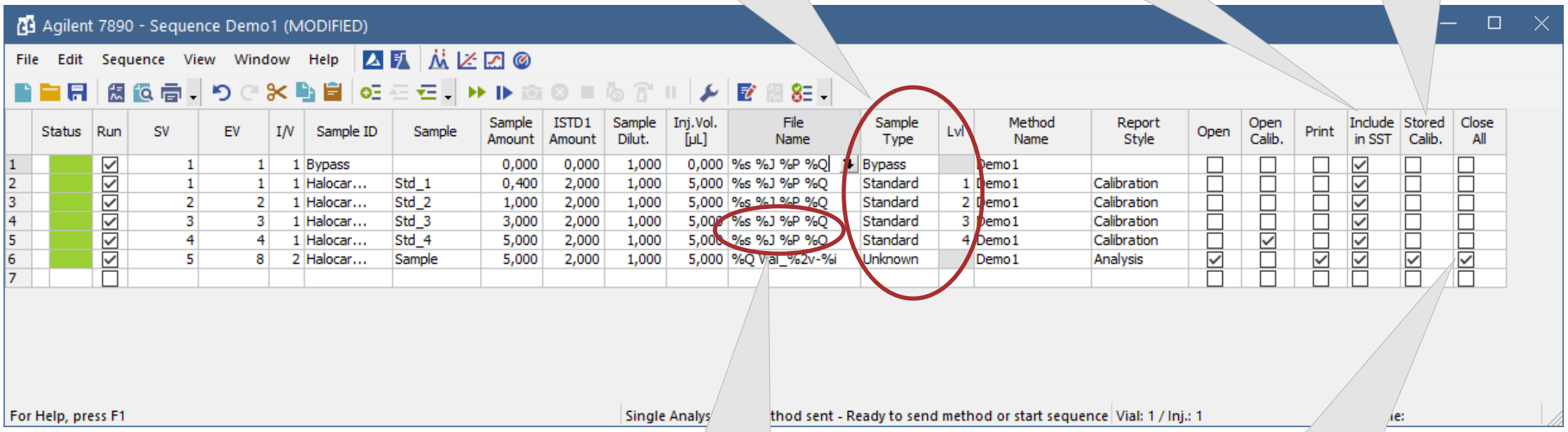
Stop sequence will stop the sequence run. Repeated Stop will stop the current analysis

Repeat Injection and Skip Vial only in active sequence

Use „Bypass“ to perform run without injection for startup and shutdown methods

Include in SST – perform SST test when injection is finished

Stored Calib. – chromatogram will be opened with stored calibration



New **file name variables**
%P – Project
%s – Sequence
%J – Method

Close All – close all currently opened chromatograms in overlay to prepare for next summary report

Pasive sequence

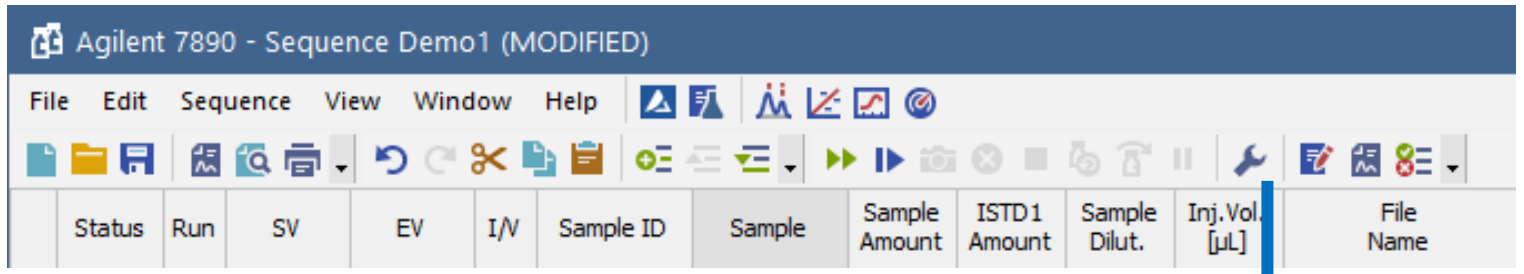
- Clarity only expects Start signal, time of analysis is set on autosampler

Active sequence

- Clarity sends a Ready signal to autosampler and waits for Start signal

AS control (Active sequence)

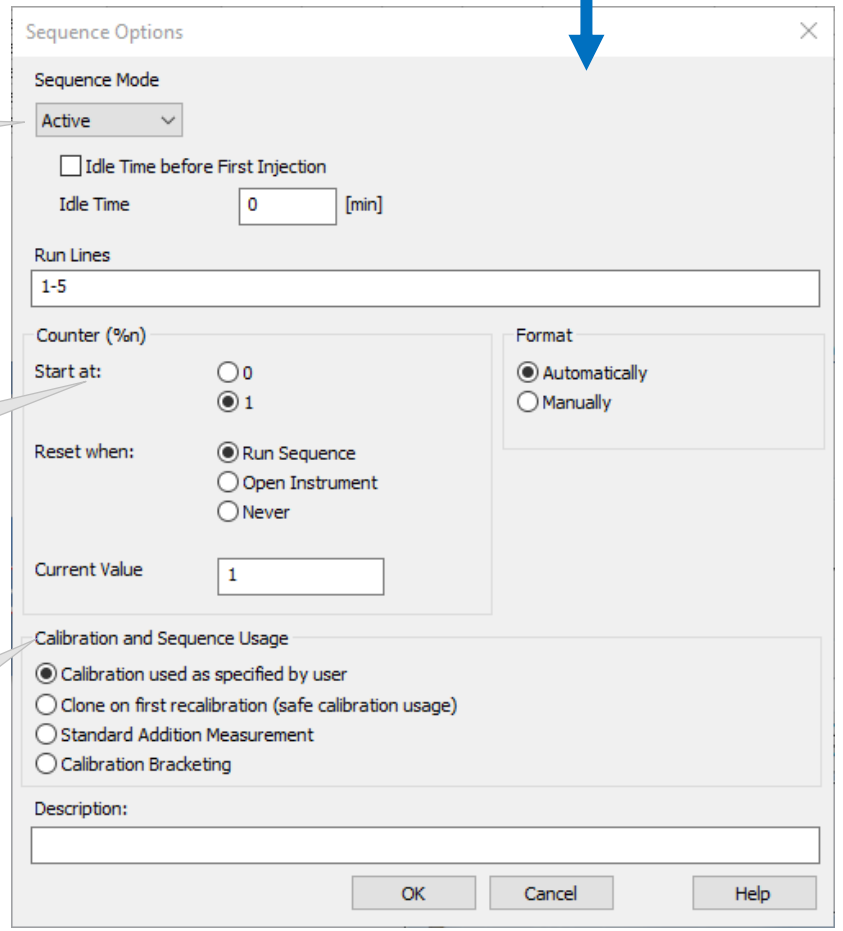
- Autosampler injects according to SV, EV, IV and Inj. Volume in sequence table

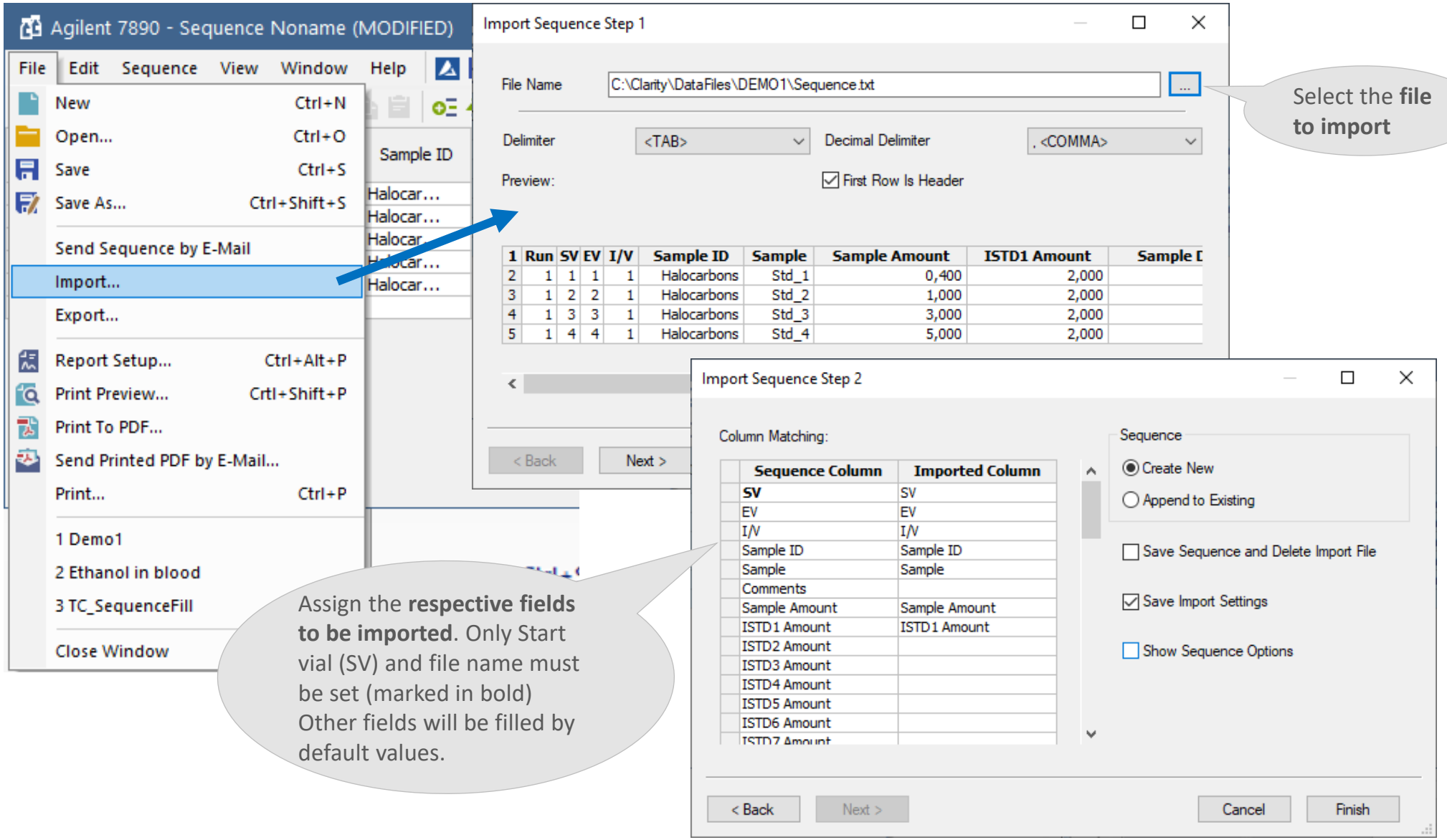


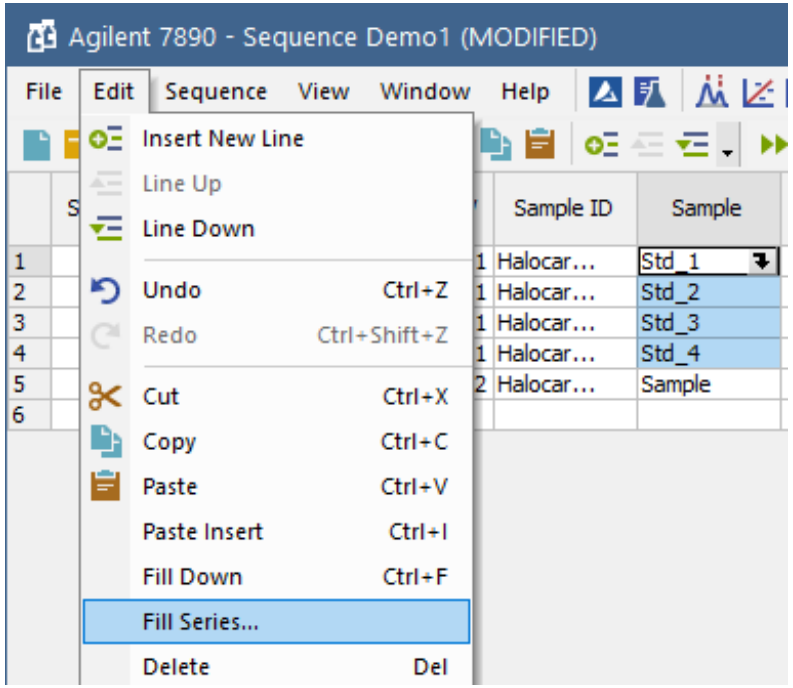
Options are:
- **Active**
- **Passive**

Initial **value for %n**

Defines mode of calibration applied for the whole sequence

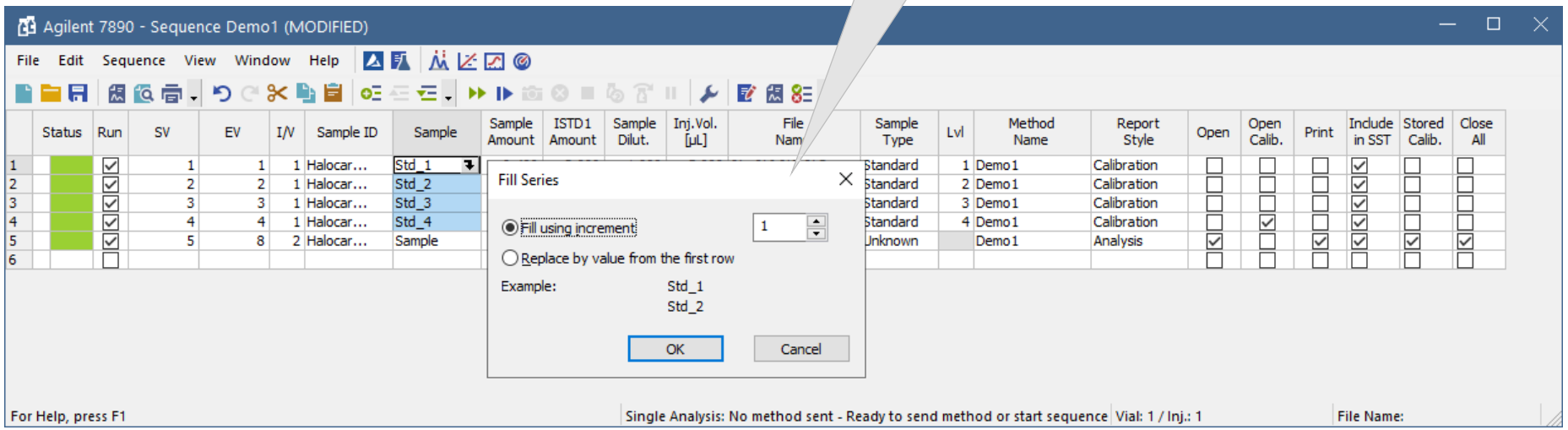



Agilent 7890 - Sequence Noname (MODIFIED)
File
Edit
Sequence
View
Window
Help
New Ctrl+N
Open... Ctrl+O
Save Ctrl+S
Save As... Ctrl+Shift+S
Send Sequence by E-Mail
Import...
Export...
Report Setup... Ctrl+Alt+P
Print Preview... Crtl+Shift+P
Print To PDF...
Send Printed PDF by E-Mail...
Print... Ctrl+P
1 Demo1
2 Ethanol in blood
3 TC_SequenceFill
Close Window
Sample ID
Halocar...
Import Sequence Step 1
File Name
C:\Clarity\DataFiles\DEMO1\Sequence.txt
...
Select the file to import
Delimiter
<TAB>
Decimal Delimiter
. <COMMA>
Preview:
First Row Is Header
1 Run SV EV I/V Sample ID Sample Sample Amount ISTD1 Amount Sample D
2 1 1 1 1 Halocarbons Std_1 0,400 2,000
3 1 2 2 1 Halocarbons Std_2 1,000 2,000
4 1 3 3 1 Halocarbons Std_3 3,000 2,000
5 1 4 4 1 Halocarbons Std_4 5,000 2,000
< Back
Next >
Import Sequence Step 2
Column Matching:
Sequence Column
Imported Column
SV SV
EV EV
I/V I/V
Sample ID Sample ID
Sample Sample
Comments
Sample Amount Sample Amount
ISTD1 Amount ISTD1 Amount
ISTD2 Amount
ISTD3 Amount
ISTD4 Amount
ISTD5 Amount
ISTD6 Amount
Sequence
Create New
Append to Existing
Save Sequence and Delete Import File
Save Import Settings
Show Sequence Options
Assign the respective fields to be imported. Only Start vial (SV) and file name must be set (marked in bold) Other fields will be filled by default values.
< Back
Next >
Cancel
Finish



- Tables - function **Fill Series...**
- In **Sequence** window
- In **Calibration** window
- **Gradient Both** numeric and text fields

Right mouse click and **Fill series command or from Edit** menu



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