DataApex

SMART SOLUTION FOR LABORATORIES

Clarity™

advanced chromatography software

# DISTRIBUTOR TRAINING

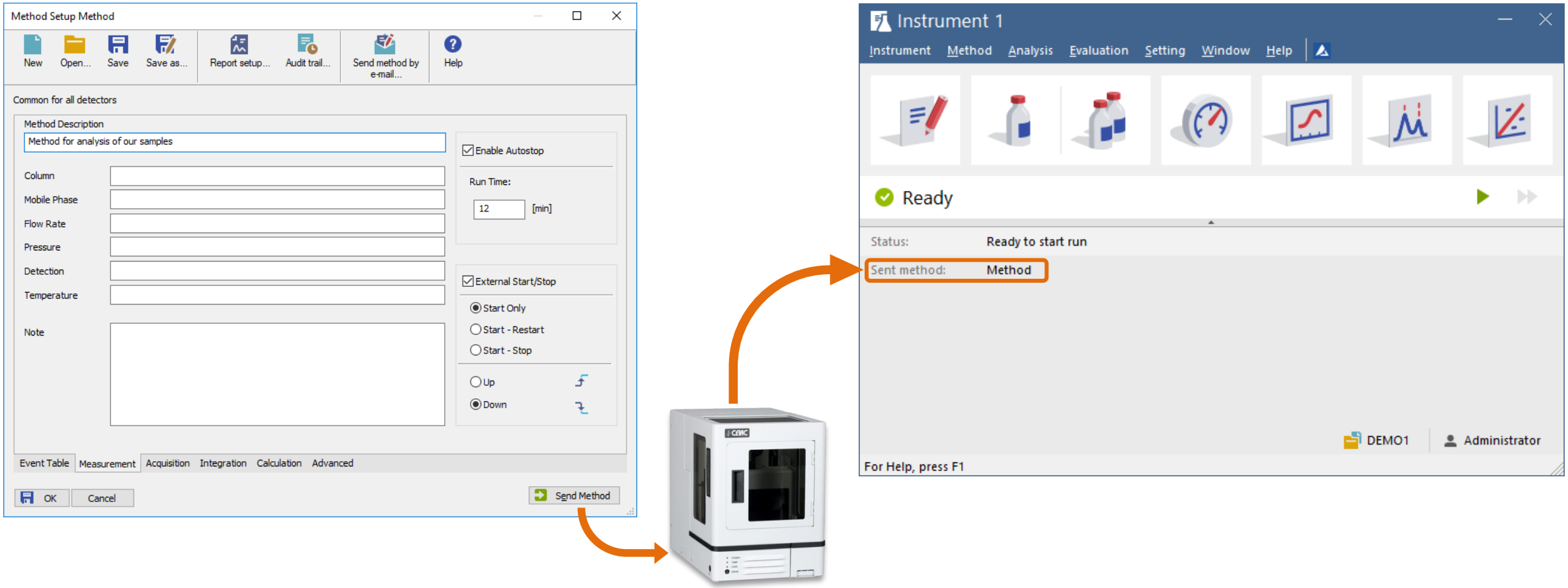
## BASIC OPERATIONS

P009/80G 10/2022

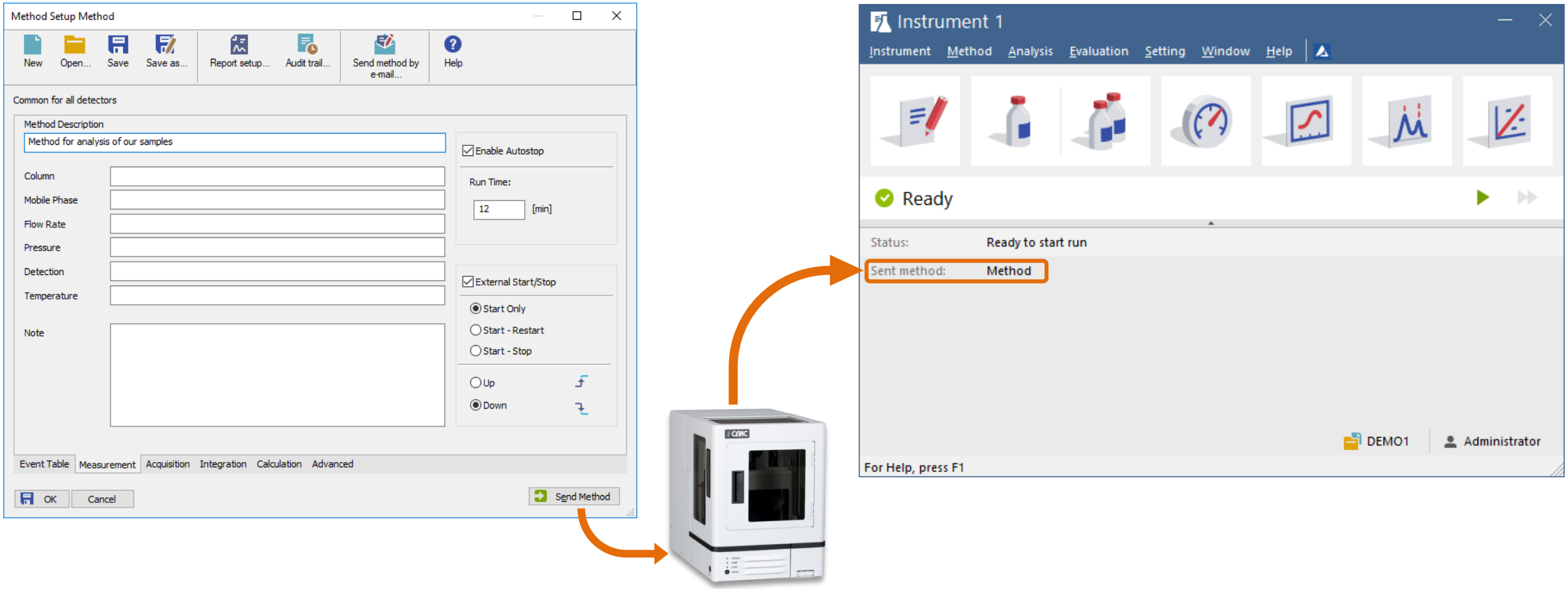
# CONTENT

- Developing a Method
- Acquiring of Data
- Creating of Calibration
- Reporting of Data

# DEVELOPING A METHOD

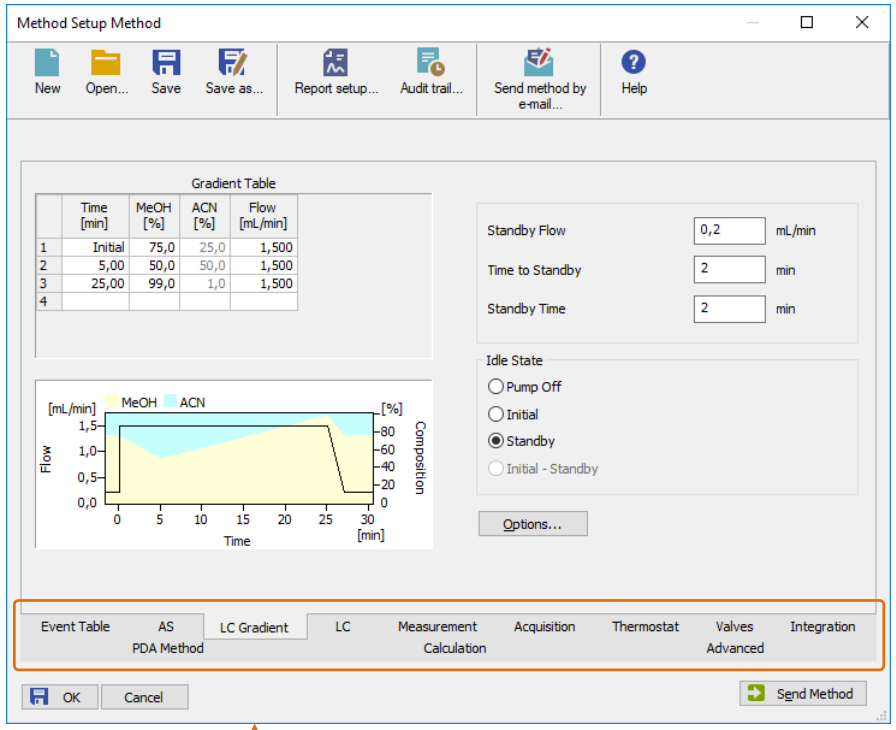


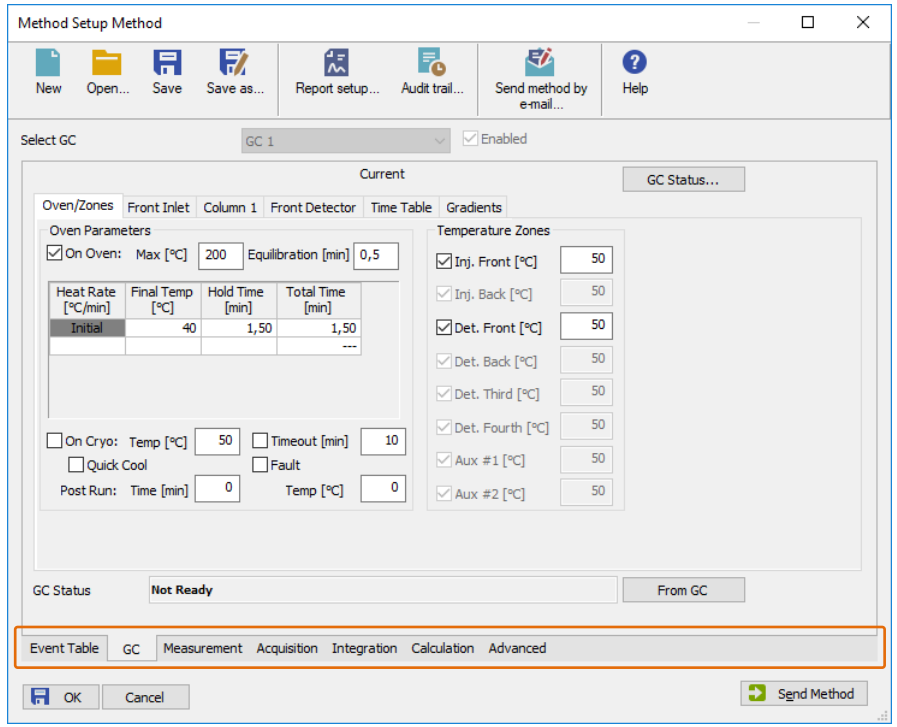
- method in Clarity = set of all instrumental parameters as well as set of processing parameters
- method opened in the Method Setup dialog can be sent to hardware and used for new acquisitions
- method is stored in method file (*.met) in current project folder

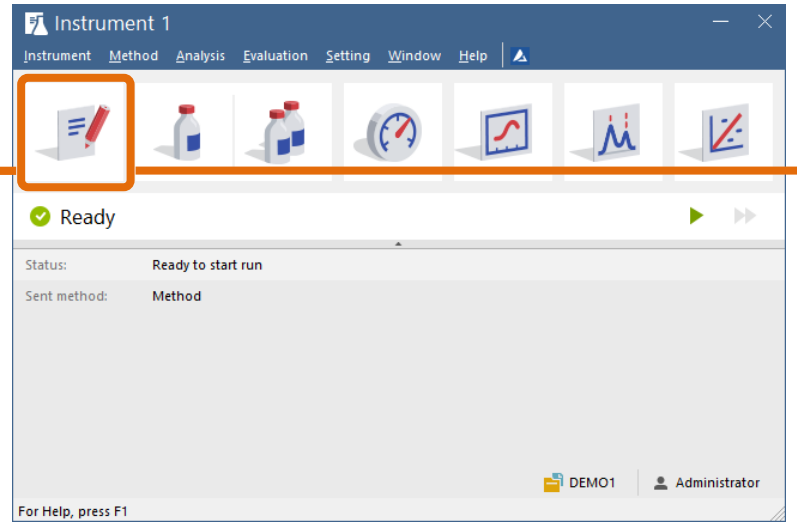


# Developing a method - proposed workflow

- Set Acquisition Parameters
- Enter Sample Information
- Acquire First Chromatogram
- Optimize Automated Integration Parameters in Method
- Store Method for Future Analyses



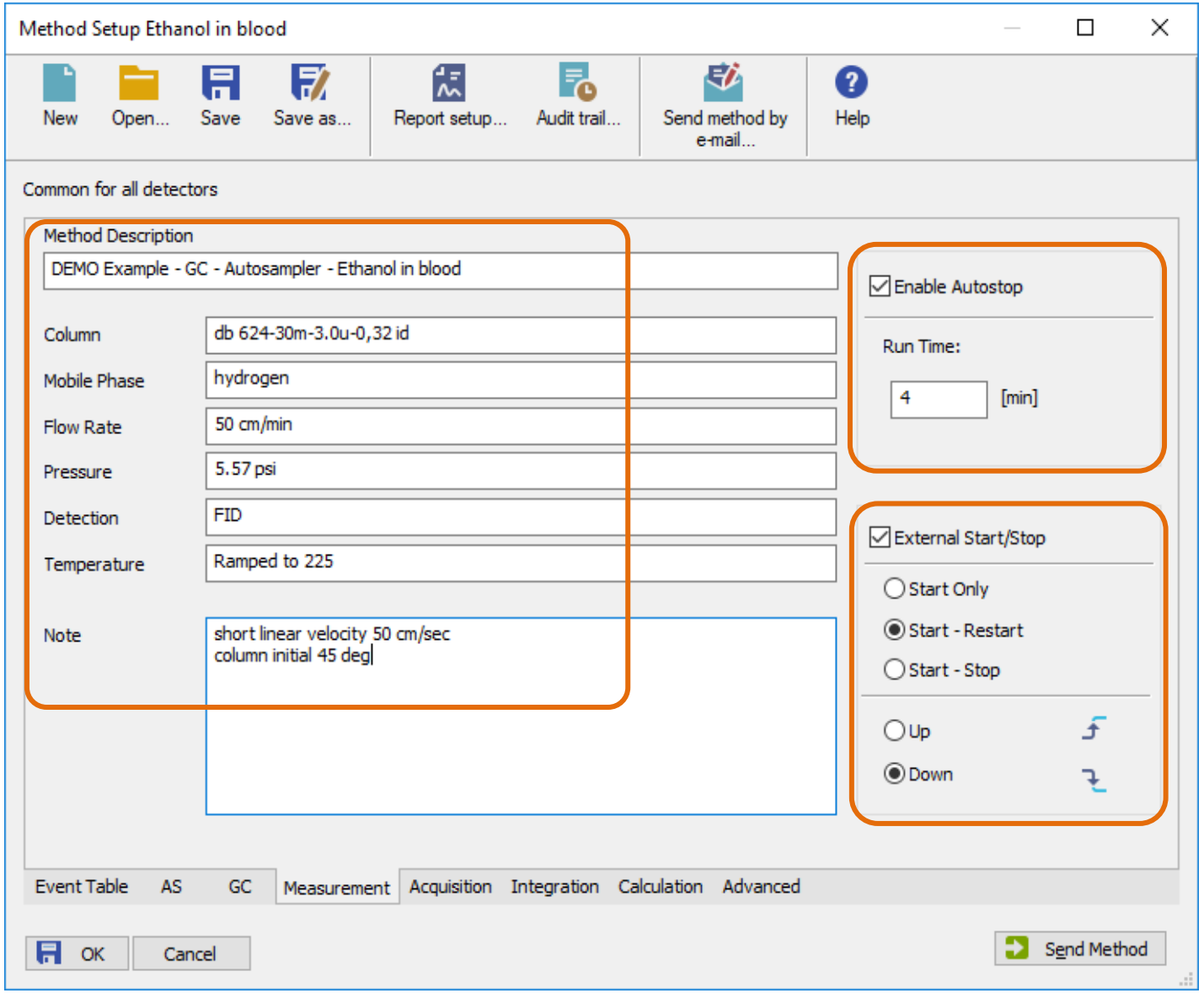

## Accessing of Method Setup Dialog

## Method Description

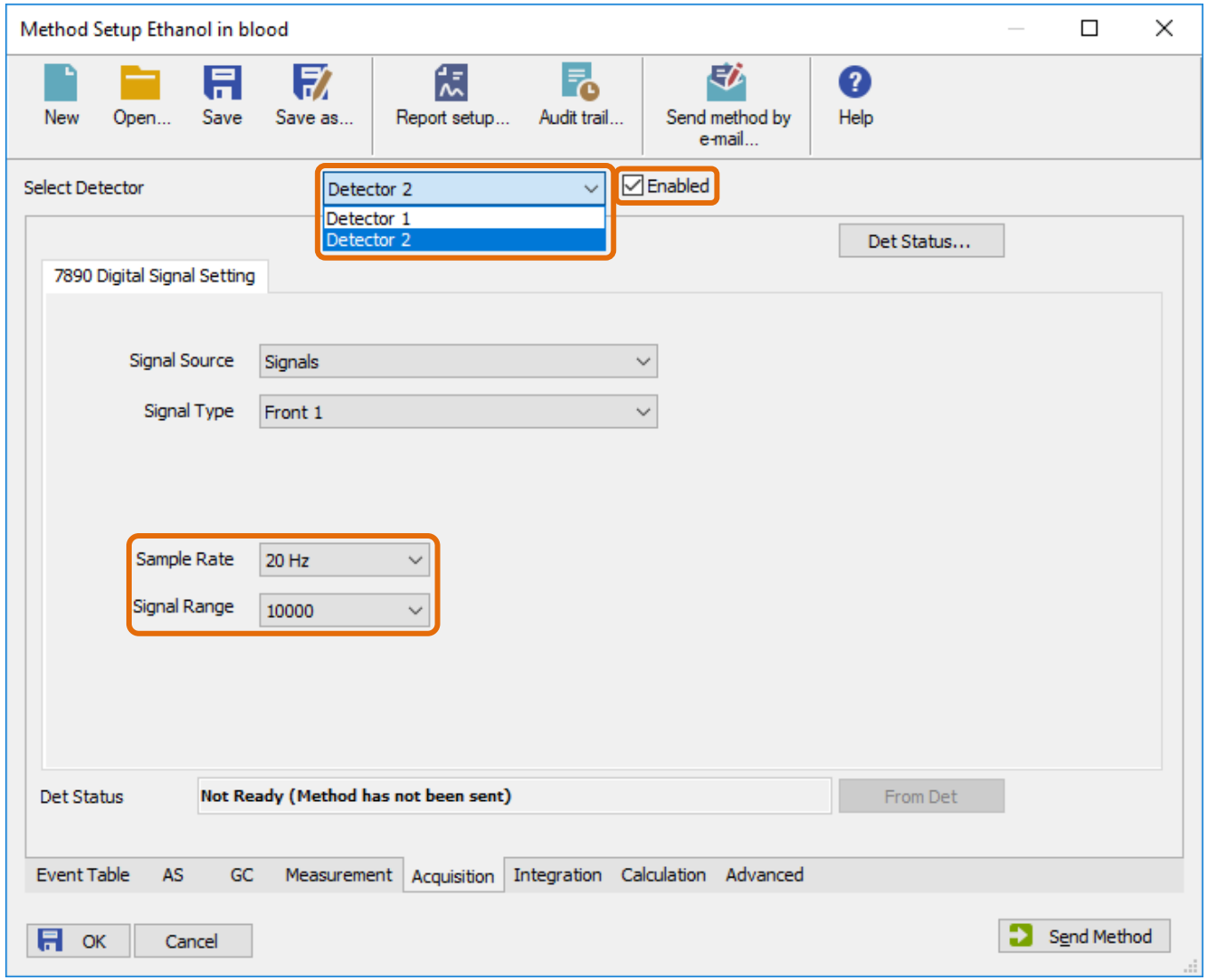
- informative

## Autostop & Run Time

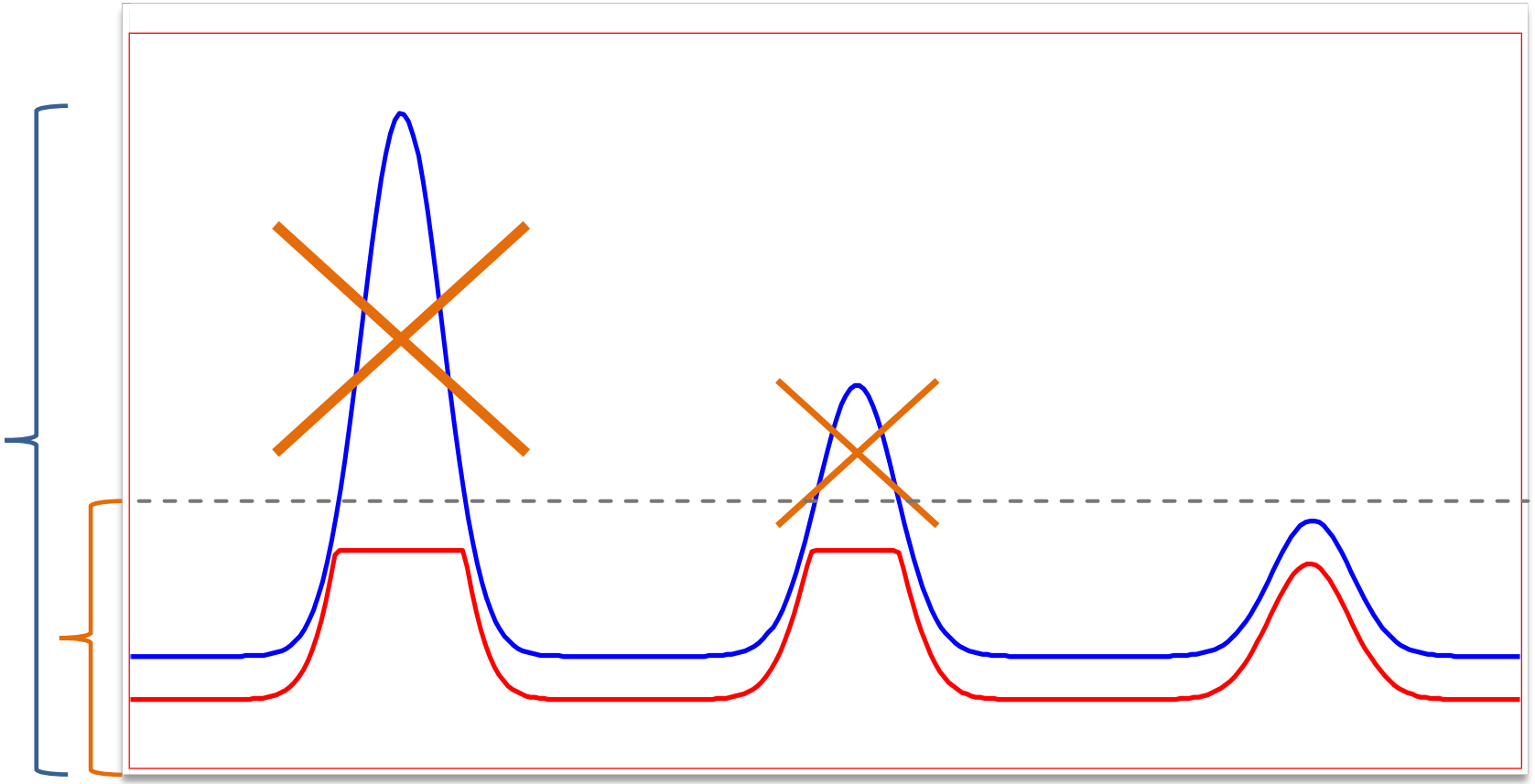
## External Start/Stop



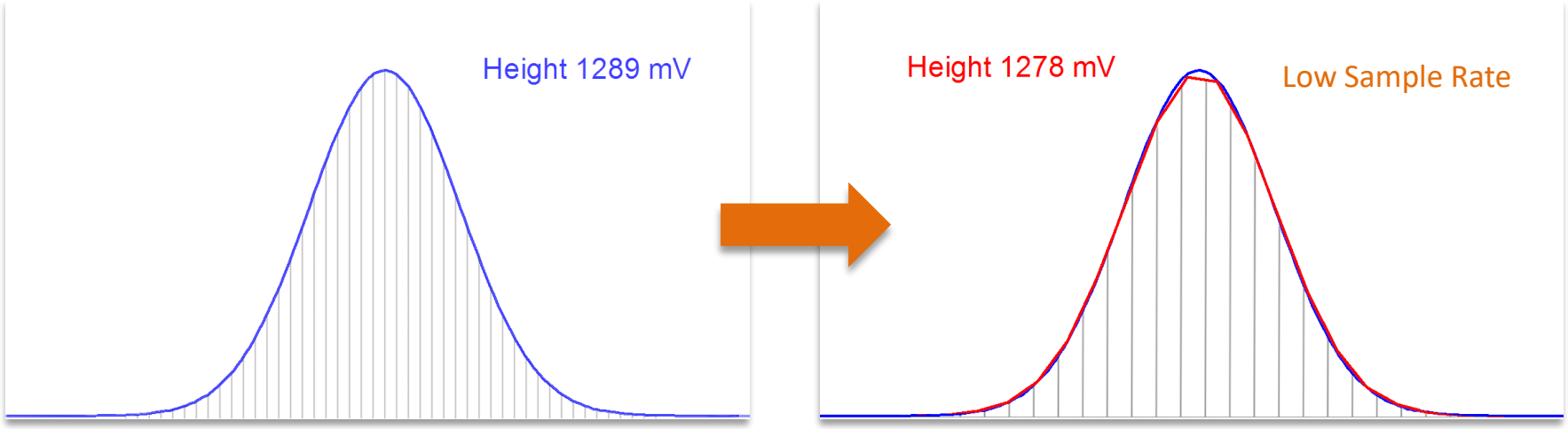
- Critical settings - they cannot be modified during acquisition
- Specific for each detector
- „Enabled“ checkbox



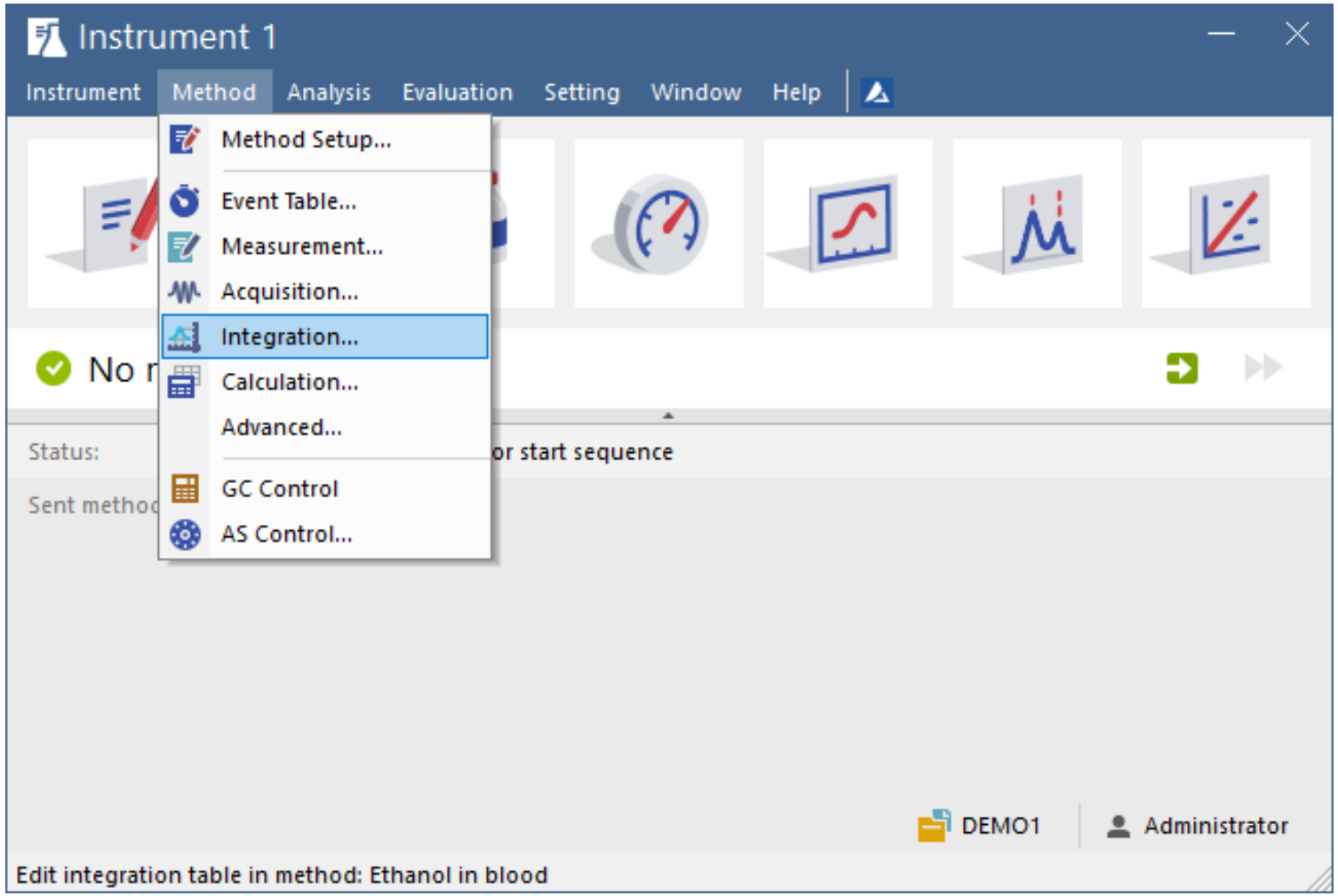
- Look dependent on configured instruments
- ‚Range' settings
- Signal outside of range → loss of chromatographic information



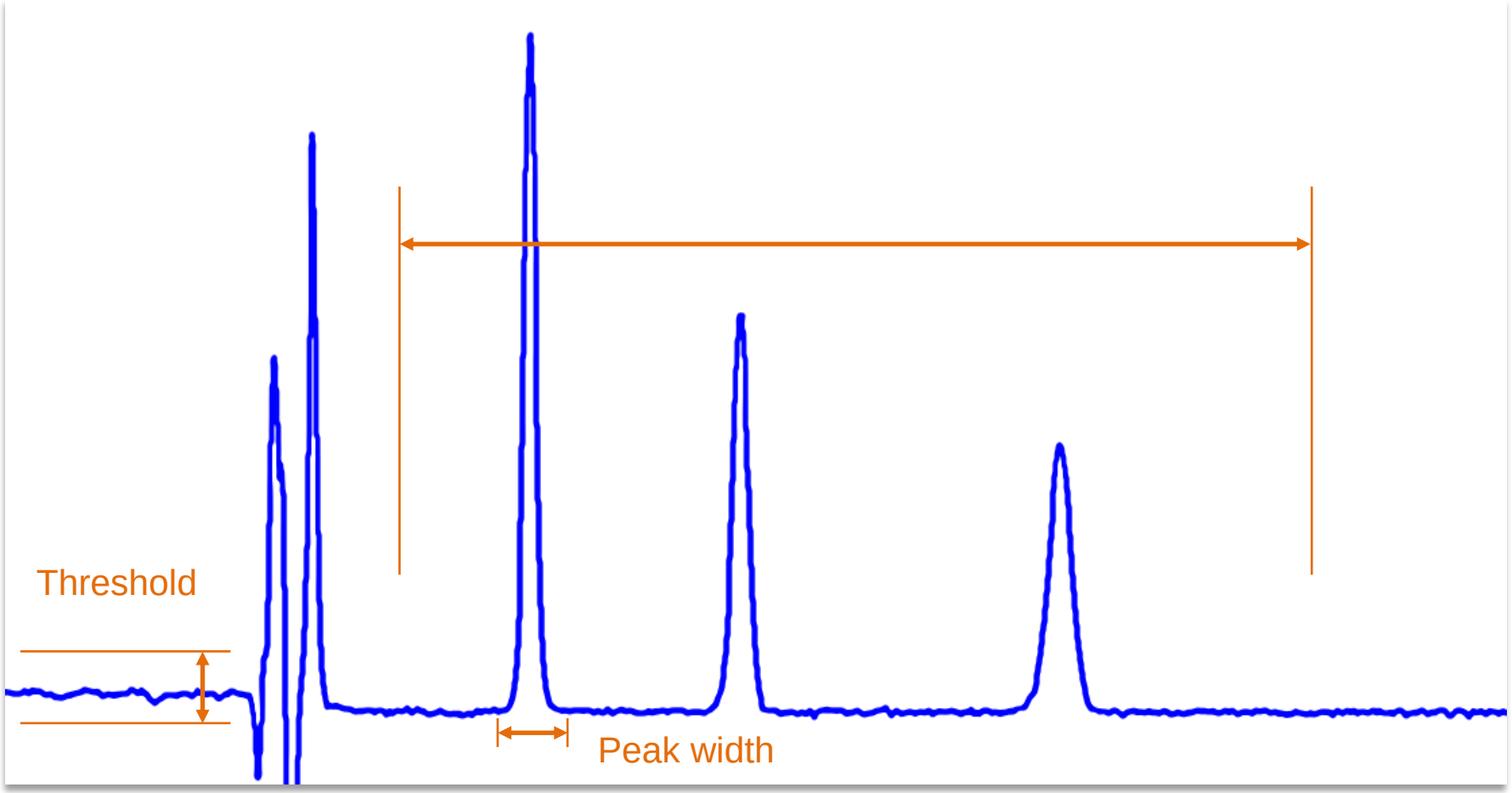
- ‚Sample rate' settings
- If it is too low, it could lead into insufficient amount of datapoints in peaks resulting in incorrect results
- Selection of correct sample rate in dependent on used HW and current analytical application
  - GC detectors - usually approx. 25-50 Hz
  - LC detectors – according to application and HW parameters
  - Spectral detectors – according to application and HW parameters



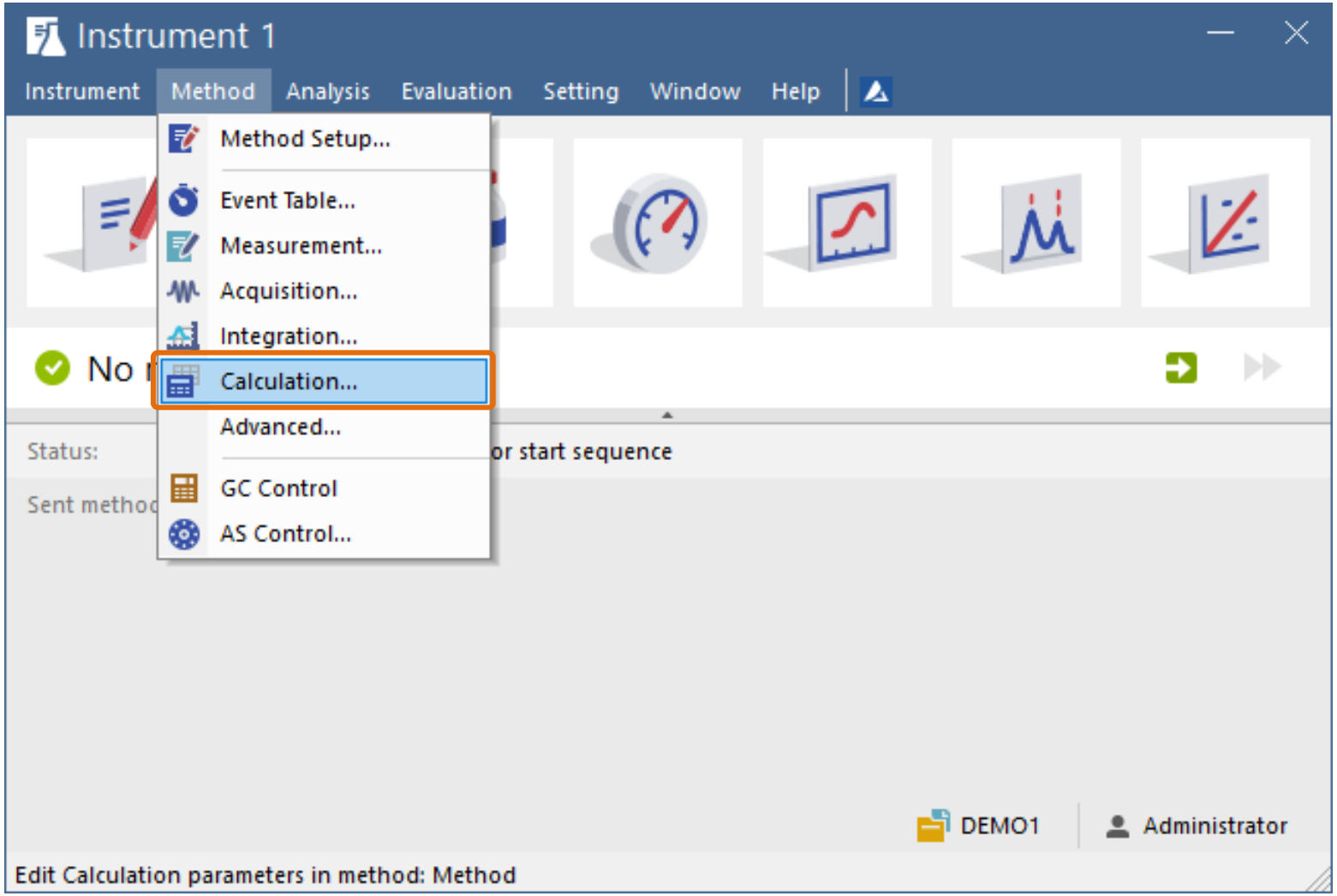
- Parameters for automatic integration of chromatogram
- Clarity integrates by default all chromatograms automatically using parameters stored in method
- If unchanged there are always applied default integration parameters originating from Clarity



- Integration parameters:
- Peak Width, Threshold, Integration Interval etc...

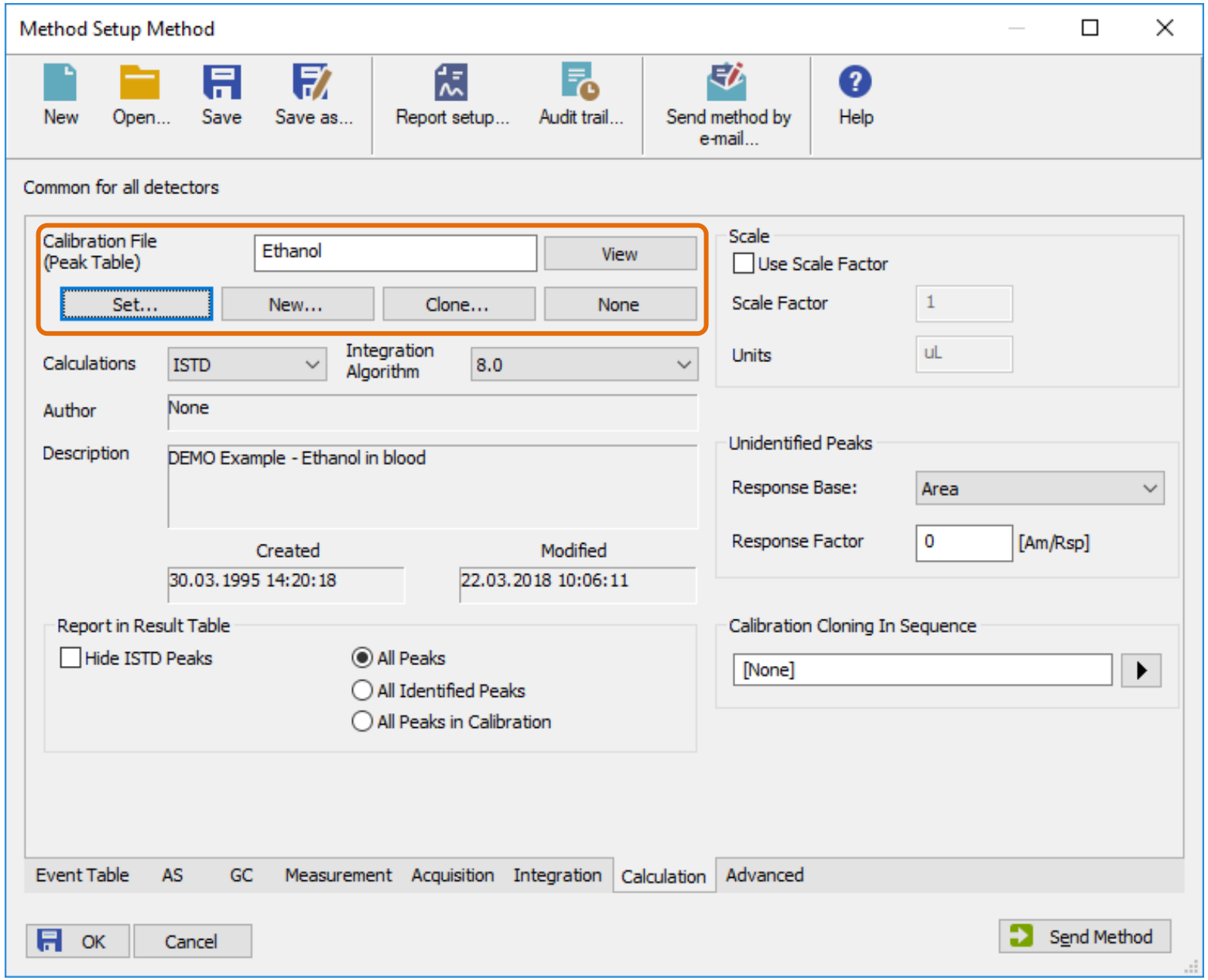


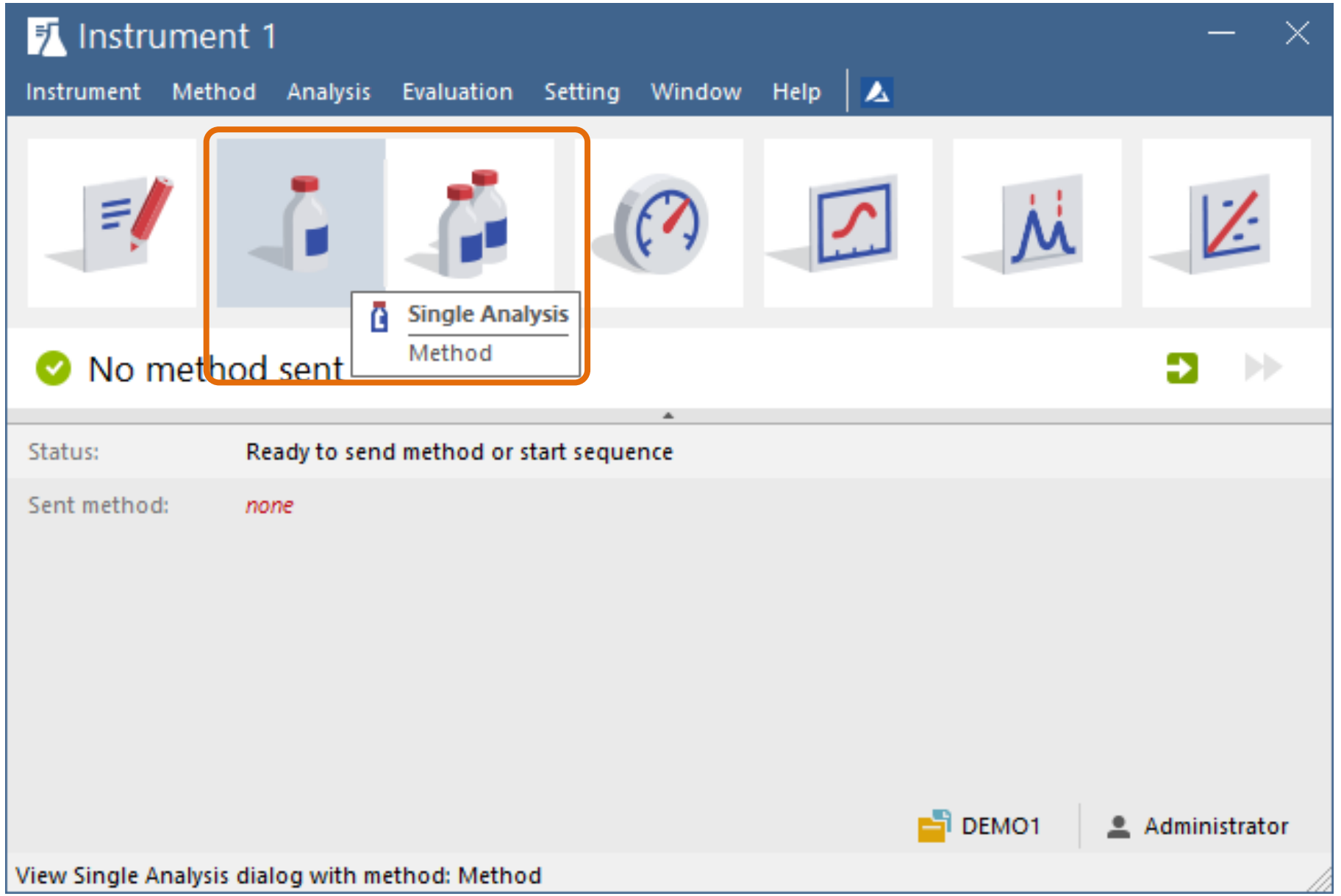
# Calculation tab



# Calculation parameters

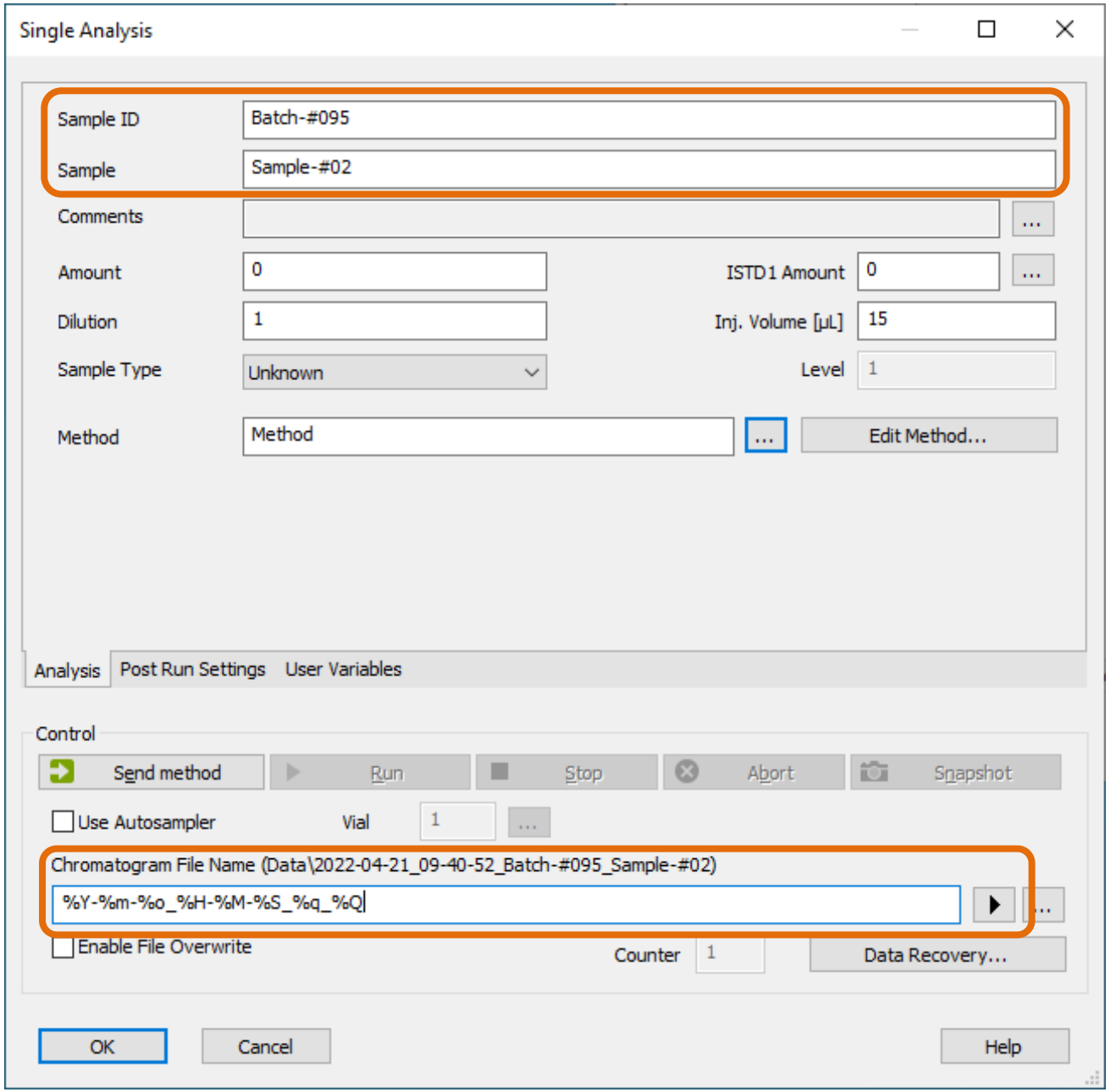
- Link the calibration file and set the calculation method



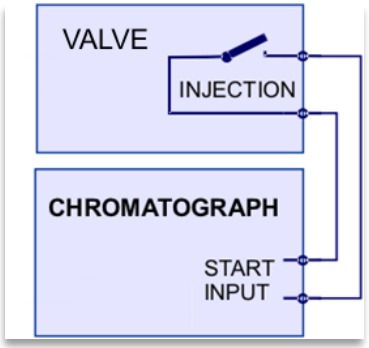

Instrument 1
Instrument
Method
Analysis
Evaluation
Setting
Window
Help
Single Analysis
Method
No method sent
Status:
Ready to send method or start sequence
Sent method:
none
DEMO1
Administrator
View Single Analysis dialog with method: Method

# Sample Information

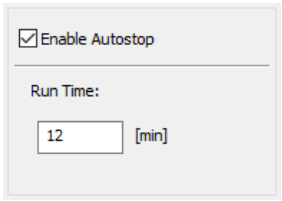
- Enter the information about the sample
- Type in the file name. You can use variables in the file name by clicking on 

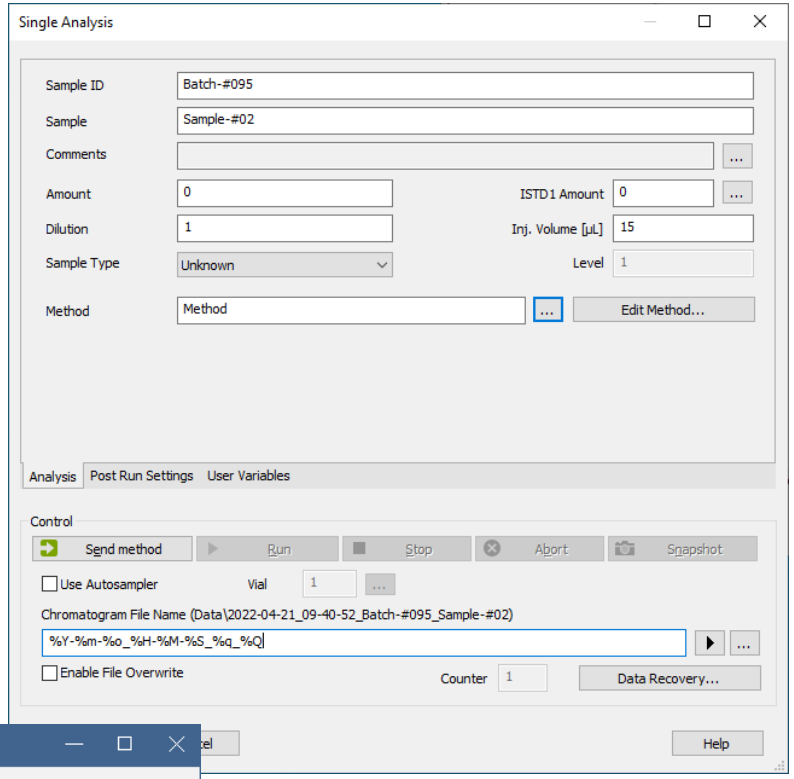


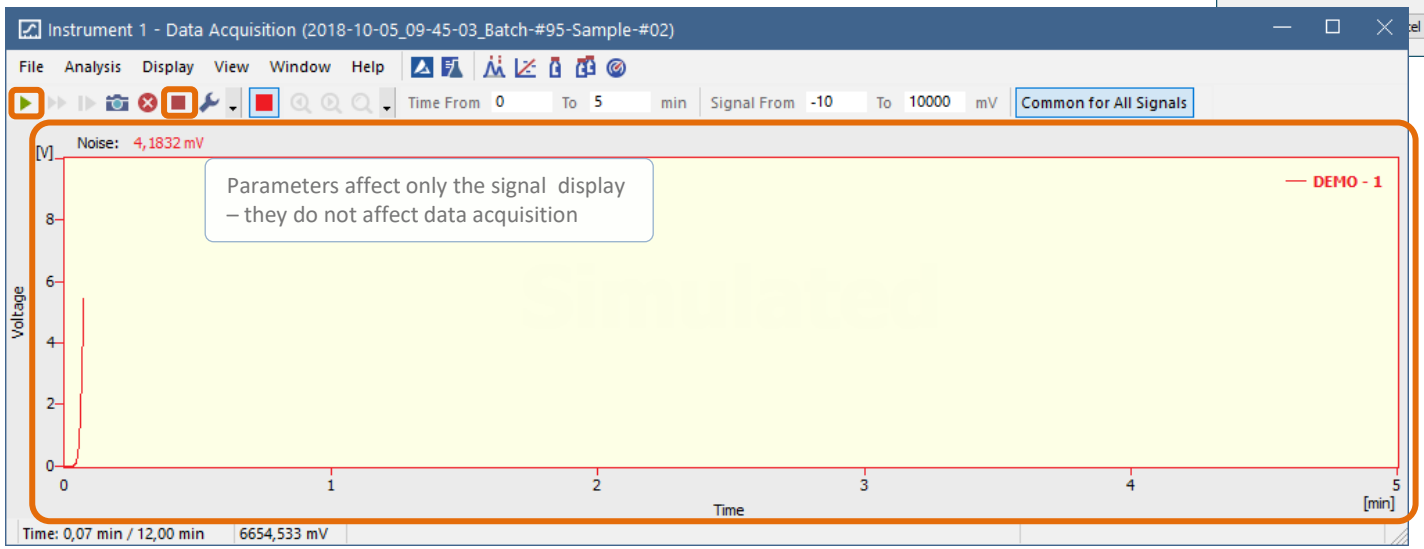
- Inject sample
  - Start data acquisition
    - Watch the signal
      - Stop acquisition





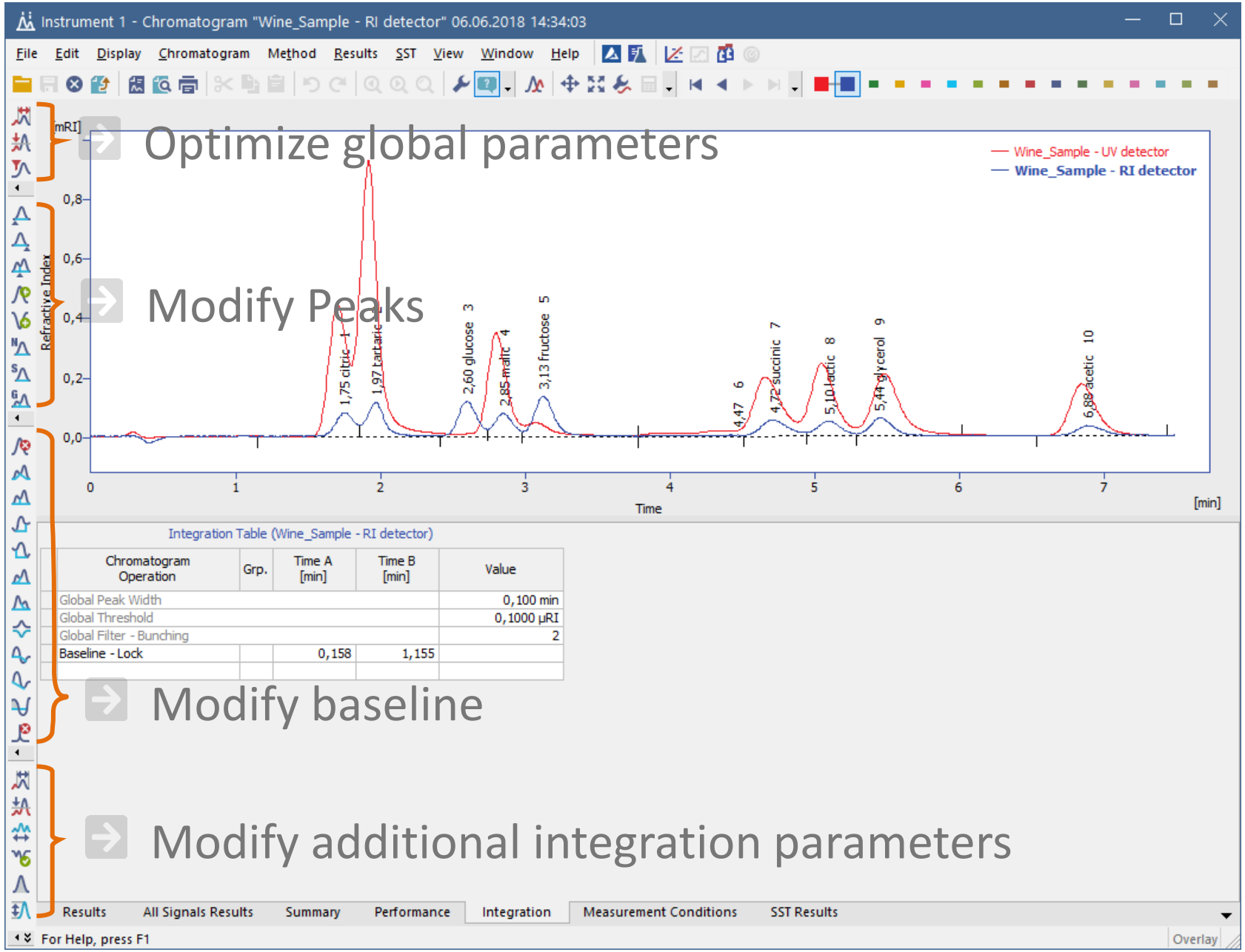


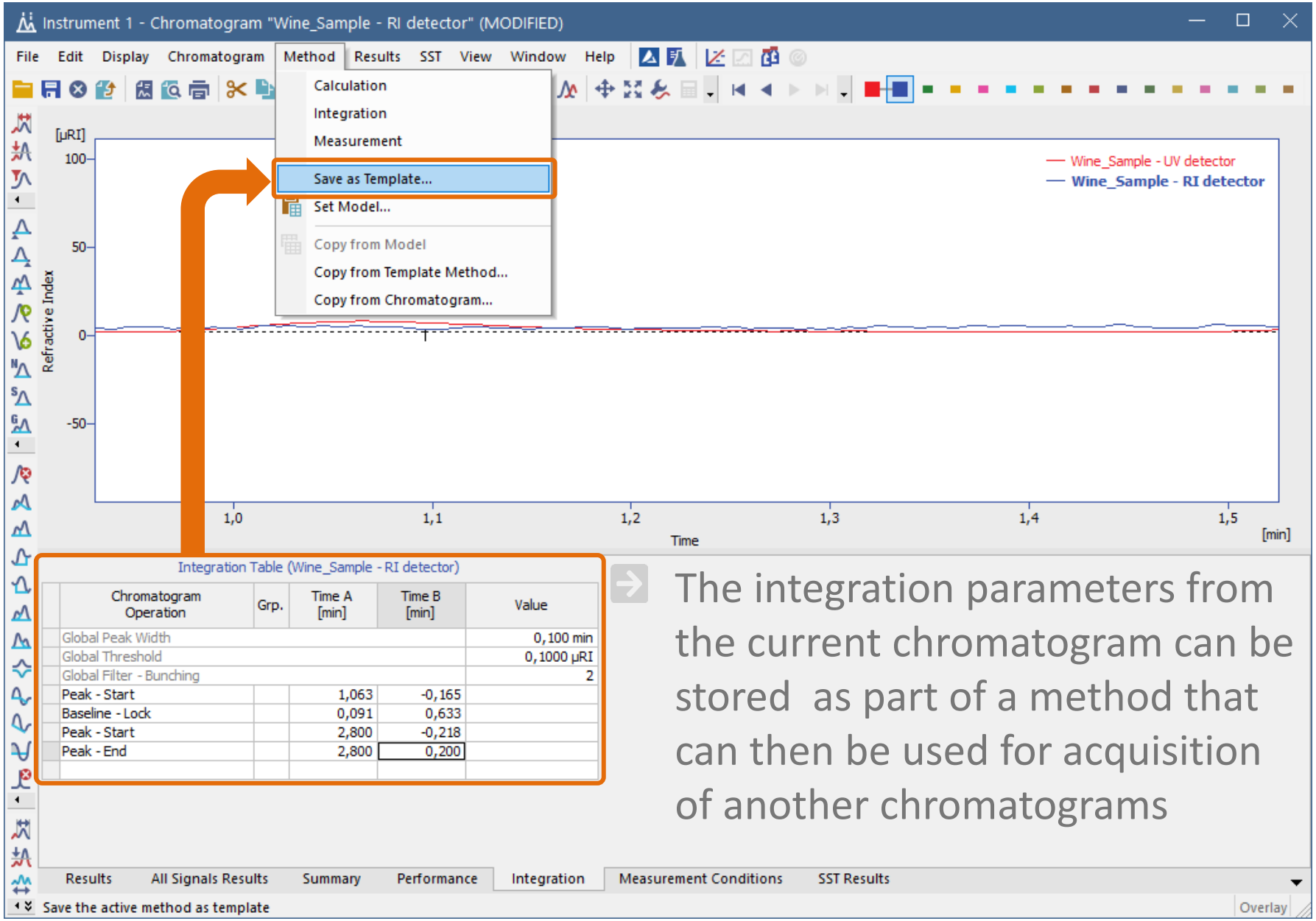



# Optimize iIntegration parameters

- For editing use graphical interface in the chromatogram window

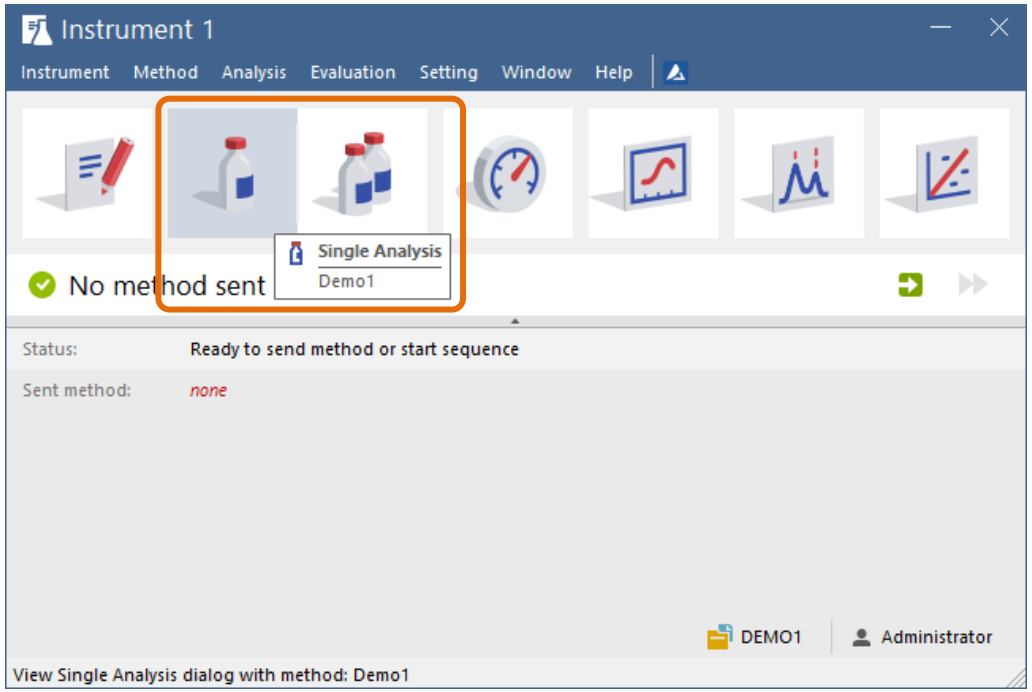


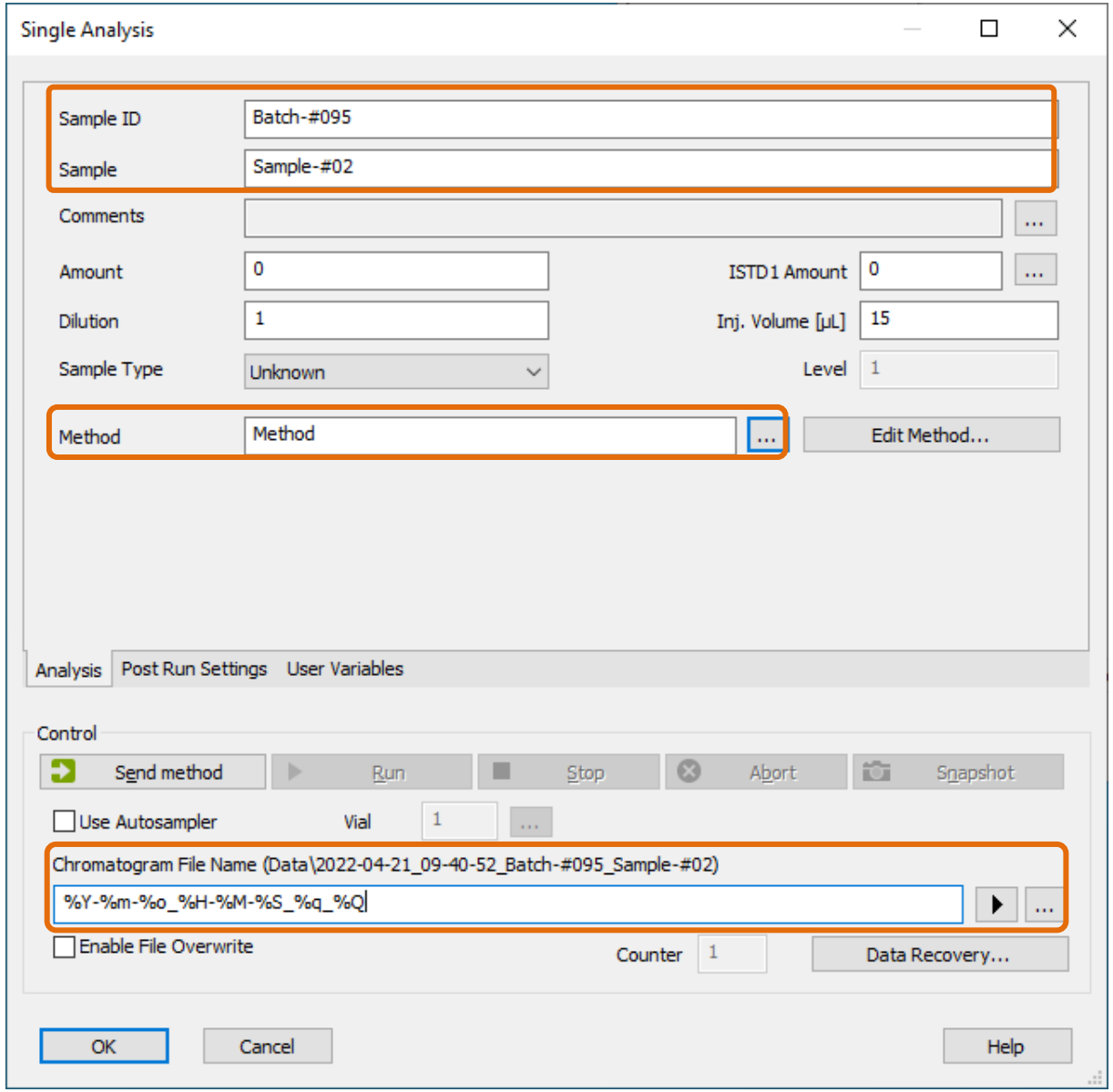



The integration parameters from the current chromatogram can be stored as part of a method that can then be used for acquisition of another chromatograms

# Single Analysis

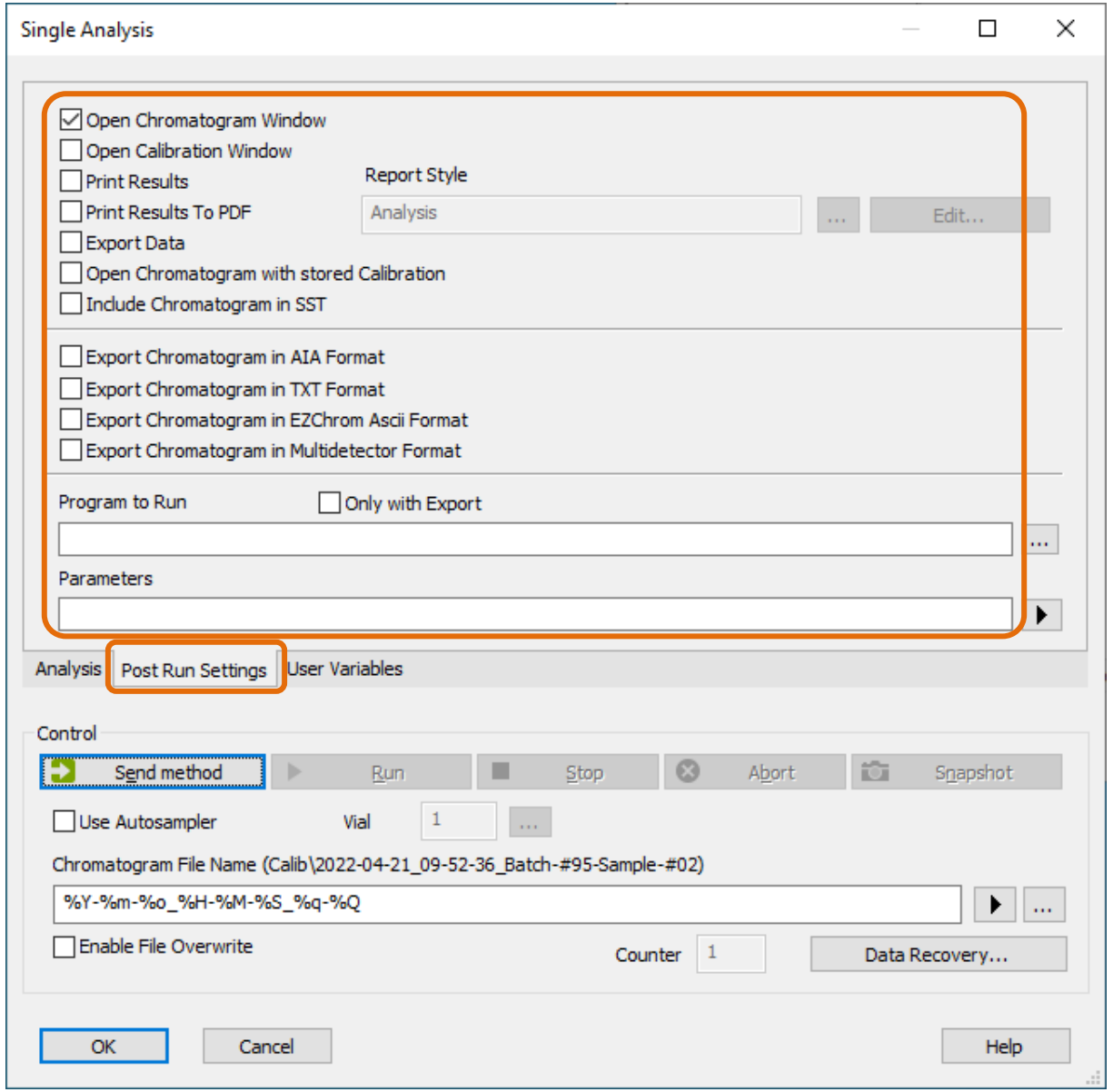
- Open Single Analysis dialog
- Select method & enter sample info



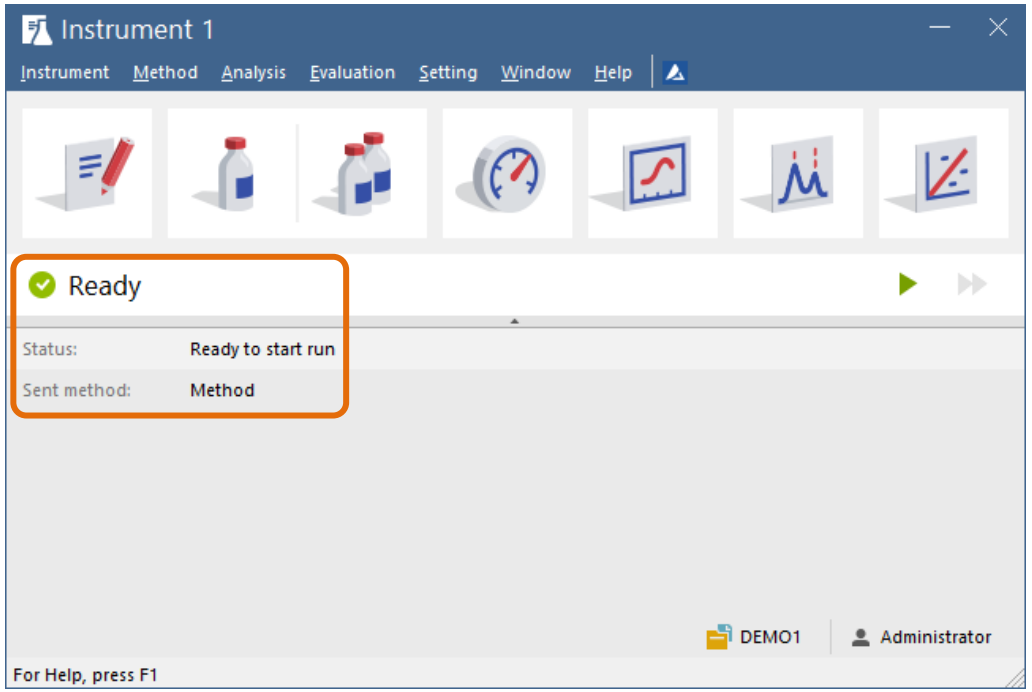
# Single Analysis

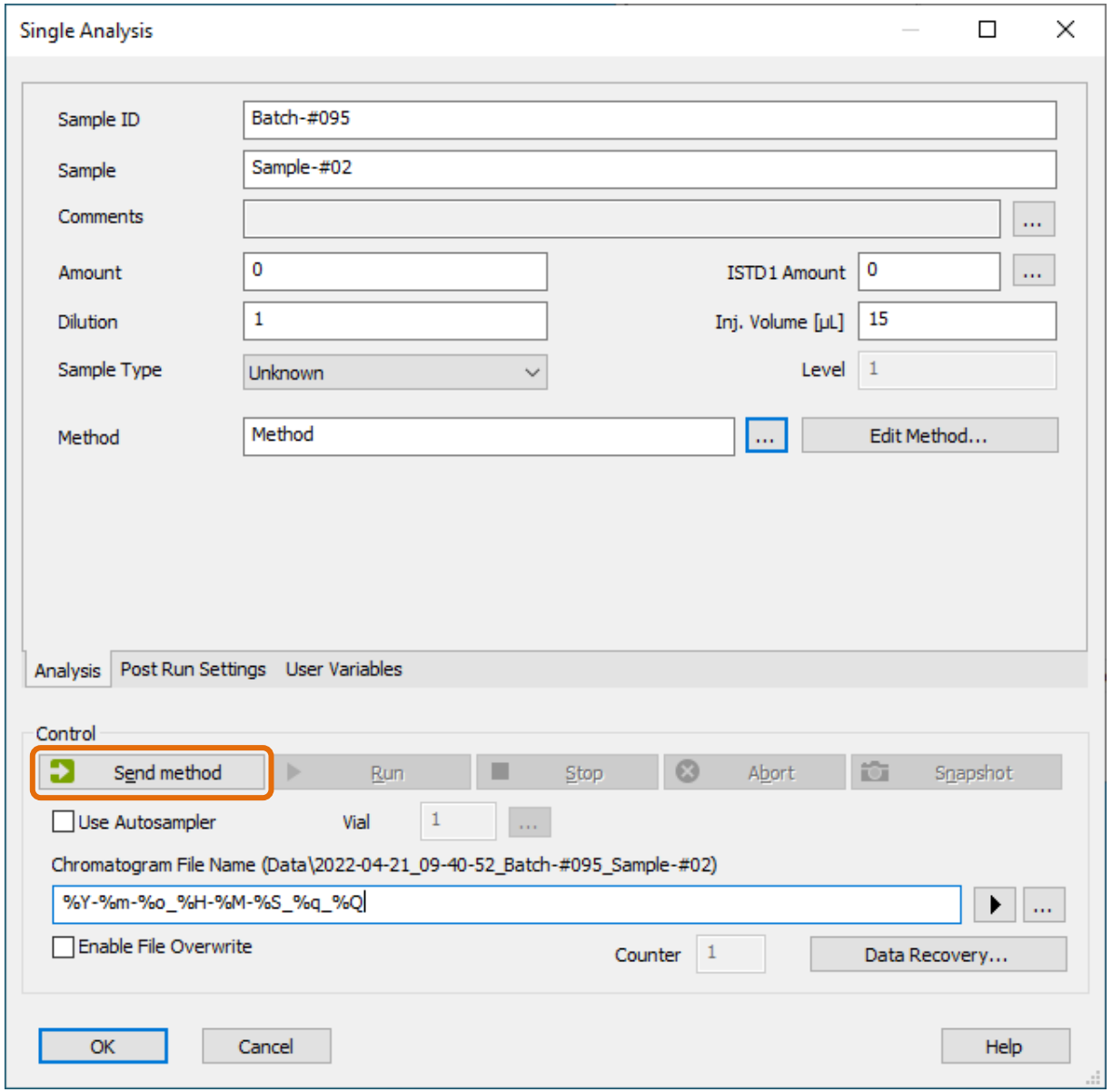
- Select default actions after finished analysis



# Single Analysis

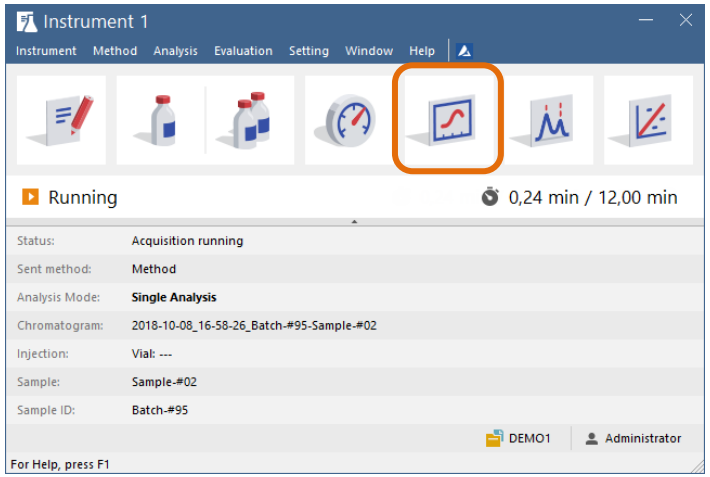
- Send a method to instrument



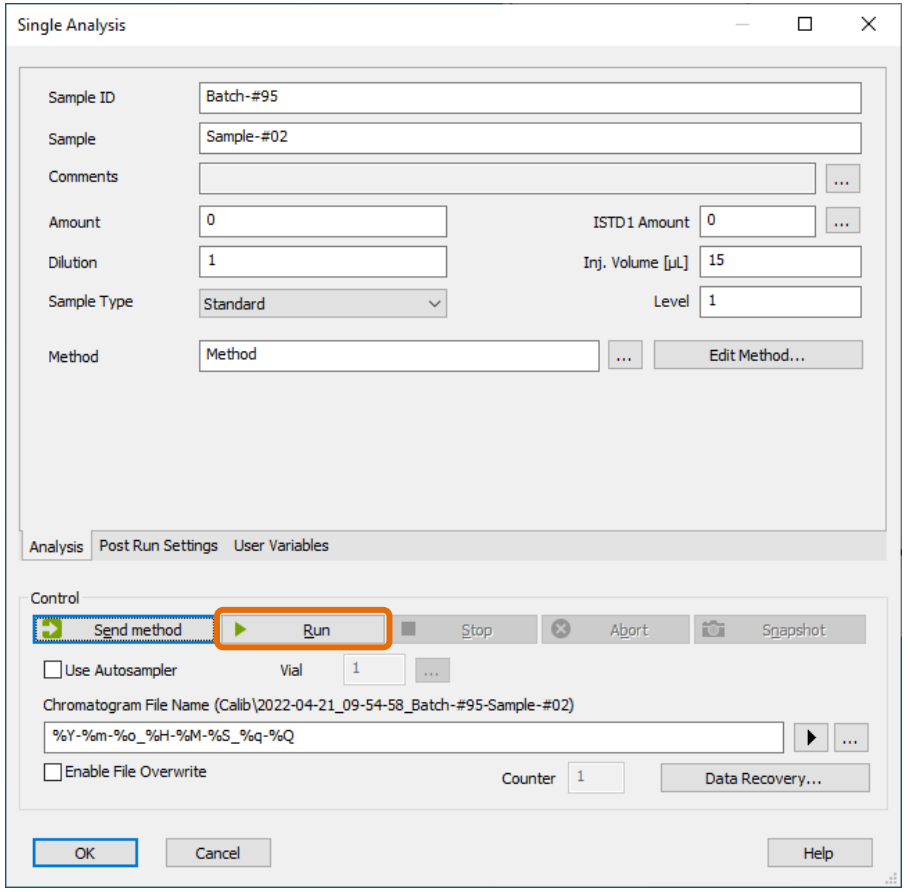



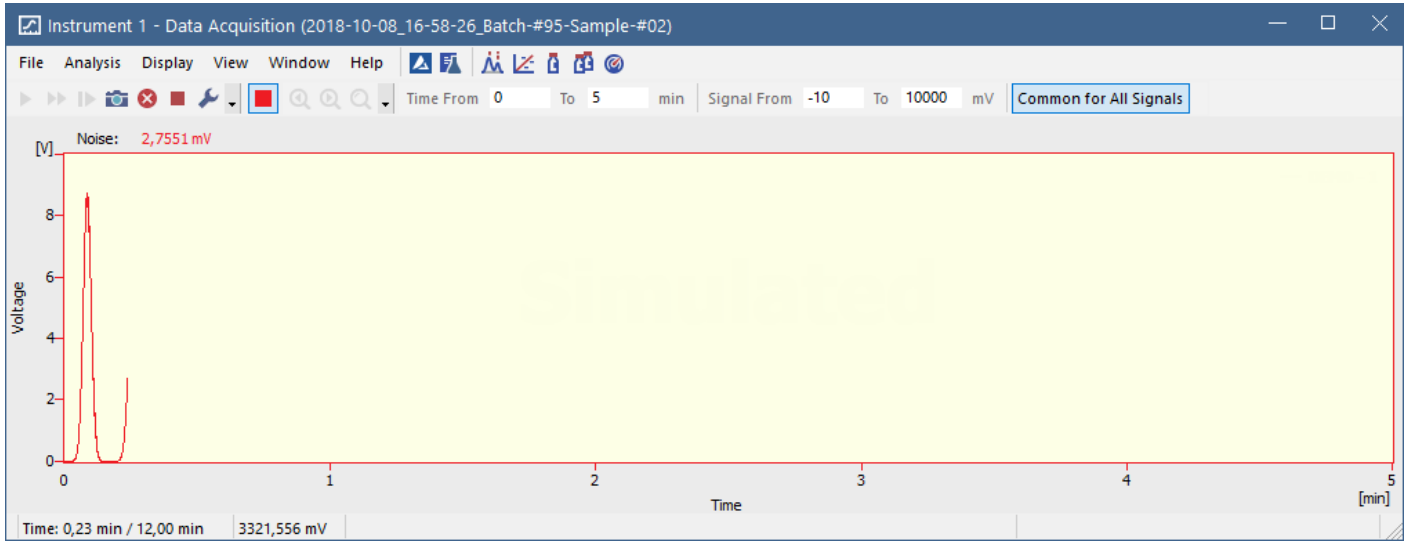
# Single Analysis

- Run Analysis & watch its progress




- Click the icon of Data Acquisition window

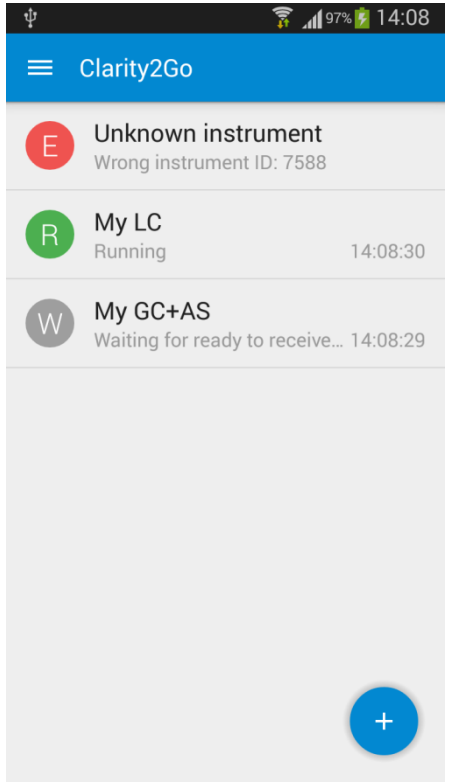


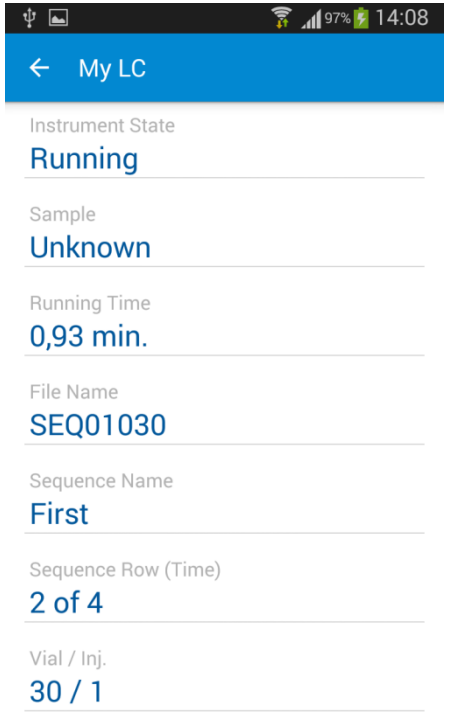




- Start & stop settings of the analysis are explained in the method development section

# Single Analysis

- Running analysis can be monitored via mobile device using Clarity2Go application

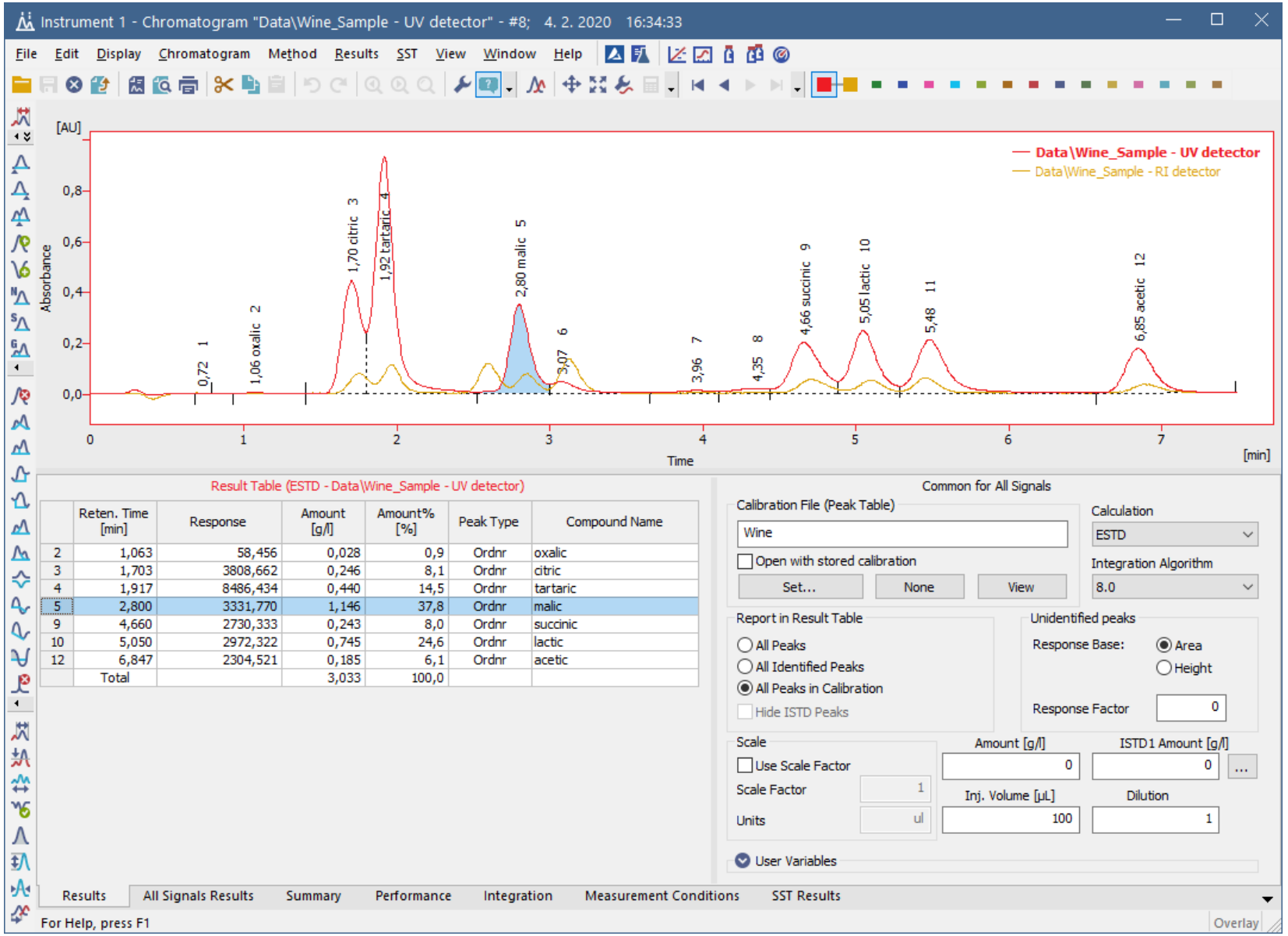


# Single Analysis

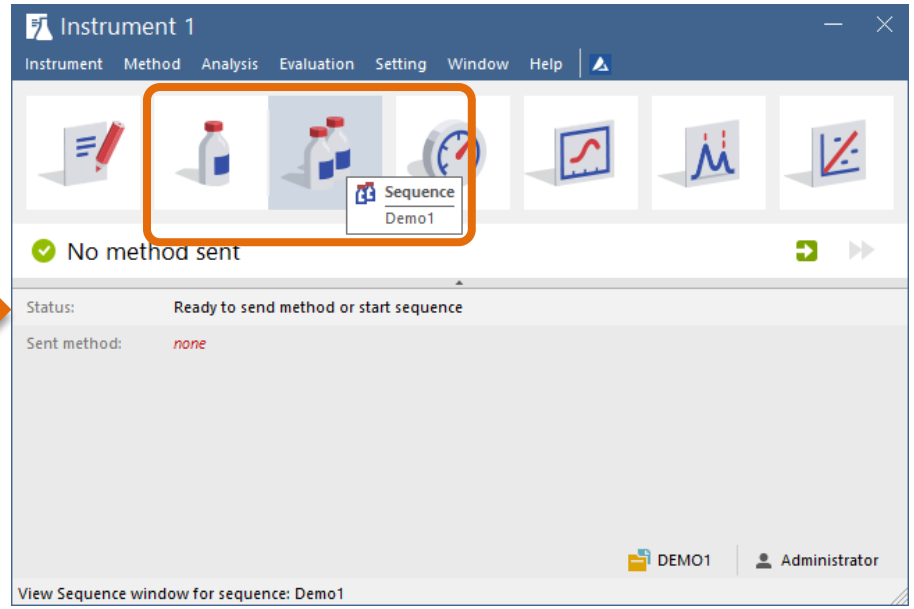
## Display results

- Open chromatogram if not set to open automatically
- Click on Results tab to display results
- Edit integration parameters, create groups of peak and/or similar
- Zoom in into graph if you wish to have a detailed section of chromatogram printed in report



# Sequence

- Analyze a large number of samples using an autosampler and the sequence option
- Sequence can be used even when injecting is performed manually

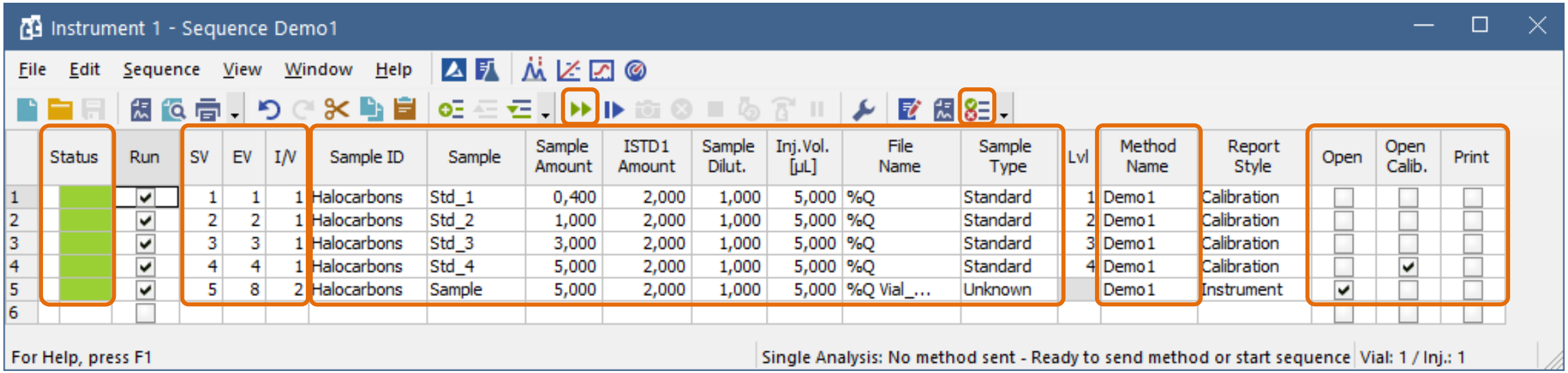


# Sequence

Enter vial info → Enter sample info → Select method → Select default actions → Check status → Start sequence

- Enter Sample ID and File Name
- Enter injection volumes for Autosampler (if used)

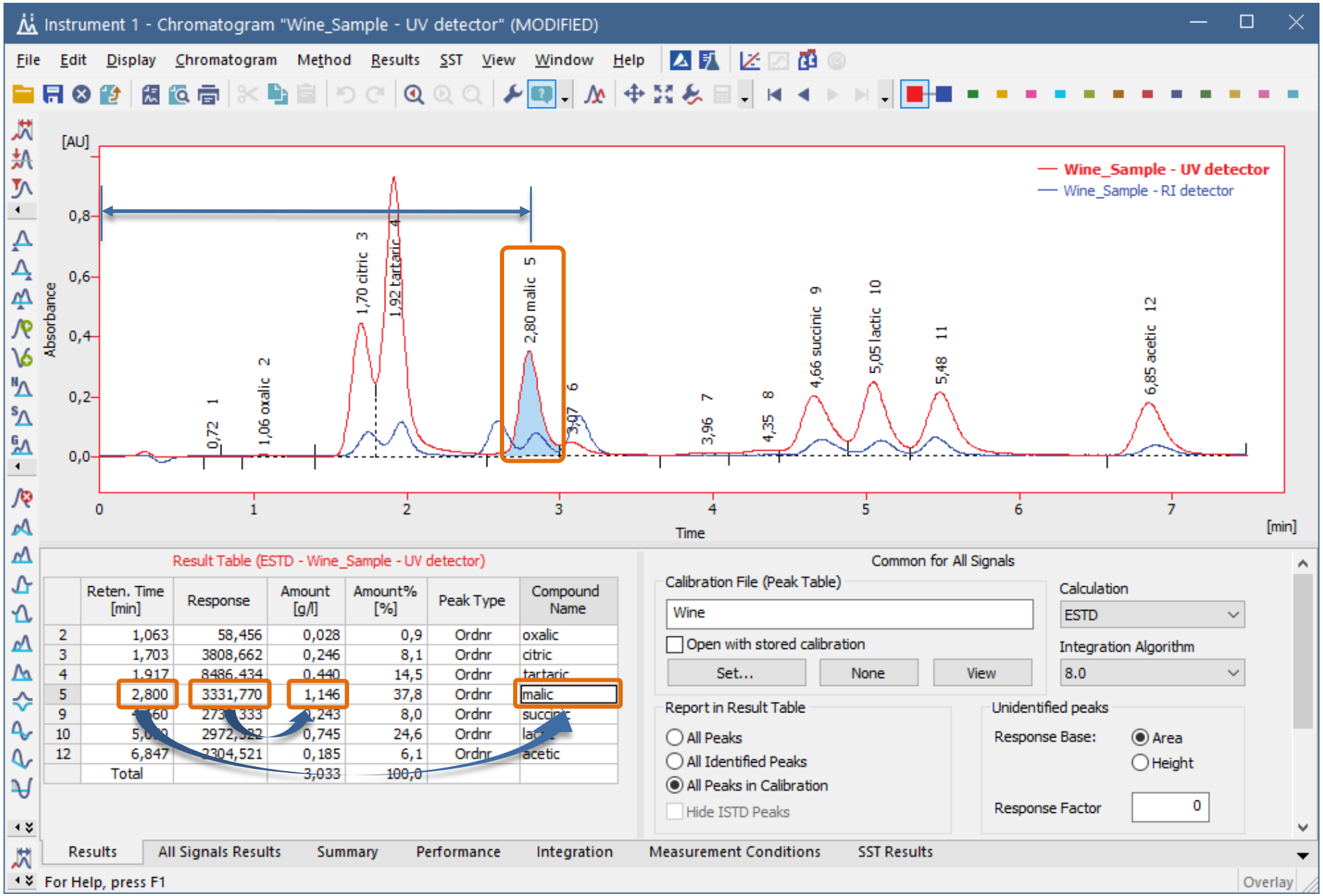
- Automated actions after each run



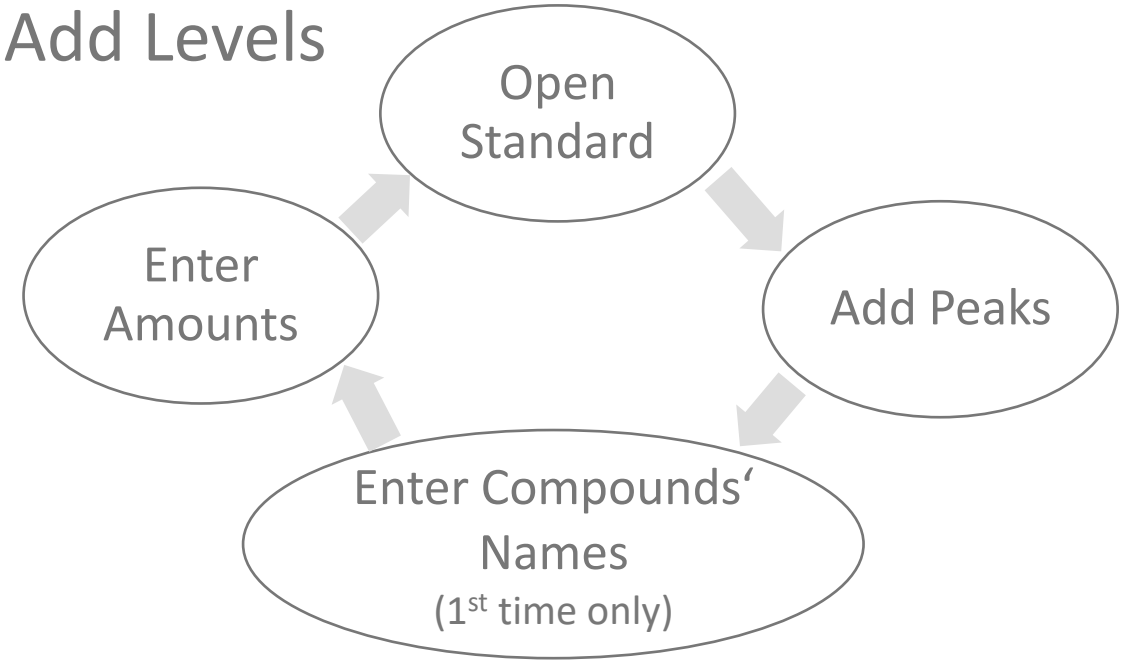

- Status Ready or with errors
- Start Vial, End Vial and number of injections per Vial
- Select a method

# Creating a calibration

- Calibration is stored in calibration file
- Allows us to identify a component and determine its amount in a sample by relating Retention Time (RT) & Compound Name and Response (Area or Height) & Amount
- Acquire First Chromatogram
- Optimize Automated Integration Parameters in Method
- Store Method for Future Analyses


Instrument 1 - Chromatogram "Wine_Sample - UV detector" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[AU]
Absorbance
Wine_Sample - UV detector
Wine_Sample - RI detector
1,70 citric 3
1,92 tartaric 4
2,80 malic 5
0,72 1
1,06 oxalic 2
3,97 6
3,96 7
4,35 8
4,66 succinic 9
5,05 lactic 10
5,48 11
6,85 acetic 12
Time
[min]
Result Table (ESTD - Wine_Sample - UV detector)
Reten. Time [min] | Response | Amount [g/l] | Amount% [%] | Peak Type | Compound Name
2 | 1,063 | 58,456 | 0,028 | 0,9 | Ordnr | oxalic
3 | 1,703 | 3808,662 | 0,246 | 8,1 | Ordnr | citric
4 | 1,917 | 8486,434 | 0,440 | 14,5 | Ordnr | tartaric
5 | 2,800 | 3331,770 | 1,146 | 37,8 | Ordnr | malic
9 | 4,660 | 273,333 | 0,243 | 8,0 | Ordnr | succinic
10 | 5,0[illegible] | 2972,322 | 0,745 | 24,6 | Ordnr | lactic
12 | 6,847 | 2304,521 | 0,185 | 6,1 | Ordnr | acetic
Total | | | 3,033 | 100,0 |
Common for All Signals
Calibration File (Peak Table)
Wine
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
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
For Help, press F1
Overlay

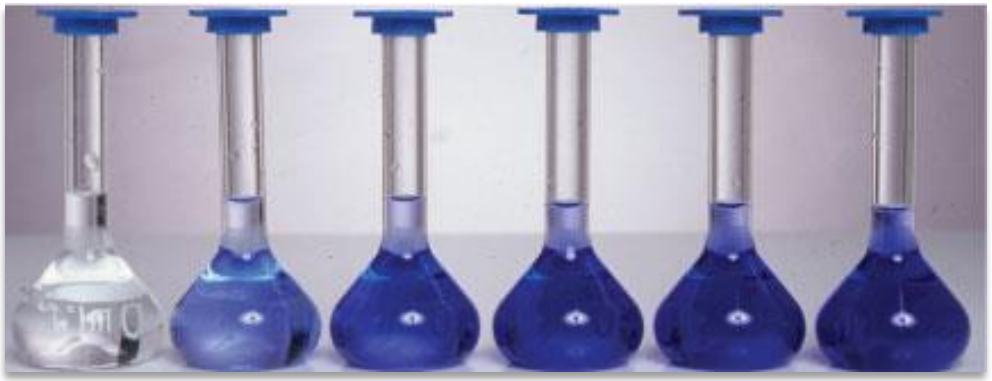
- Acquire chromatograms from known Standards
  - Set Calibration Options
    - Add Levels

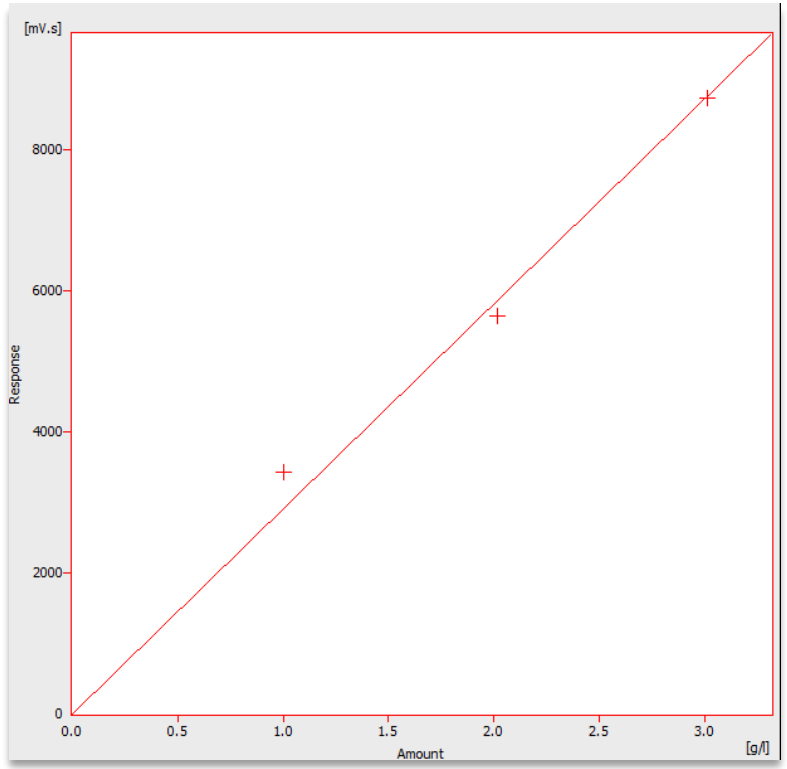



  - Save Calibration File
    - Link to Chromatogram

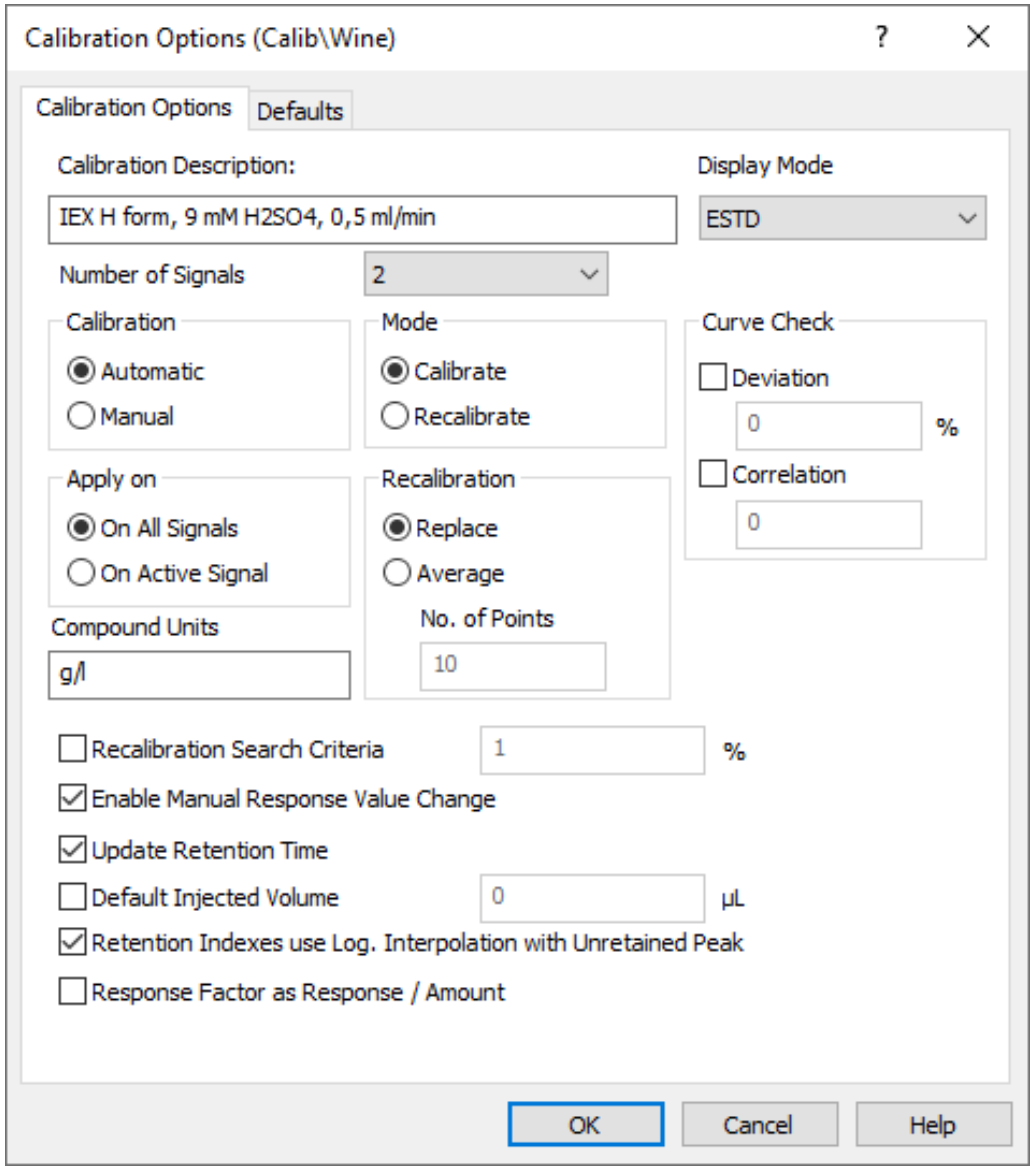
# Acquire Standards

- Acquire chromatograms of standards containing known compounds with know amounts
- Each standard will add a new point or ‚Level‘ to the calibration curve of each compound
- The calibration relates detector response to the amount of compound

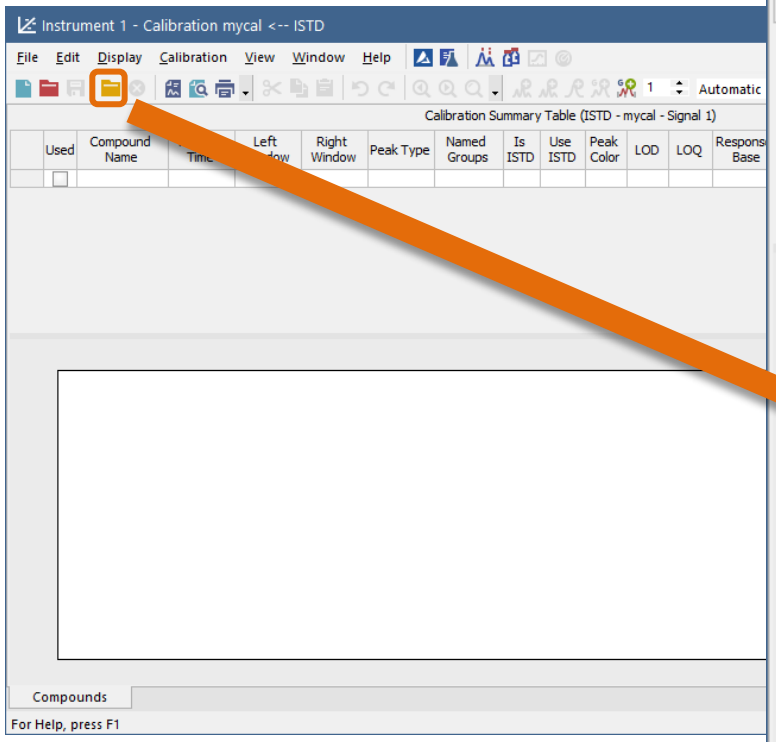


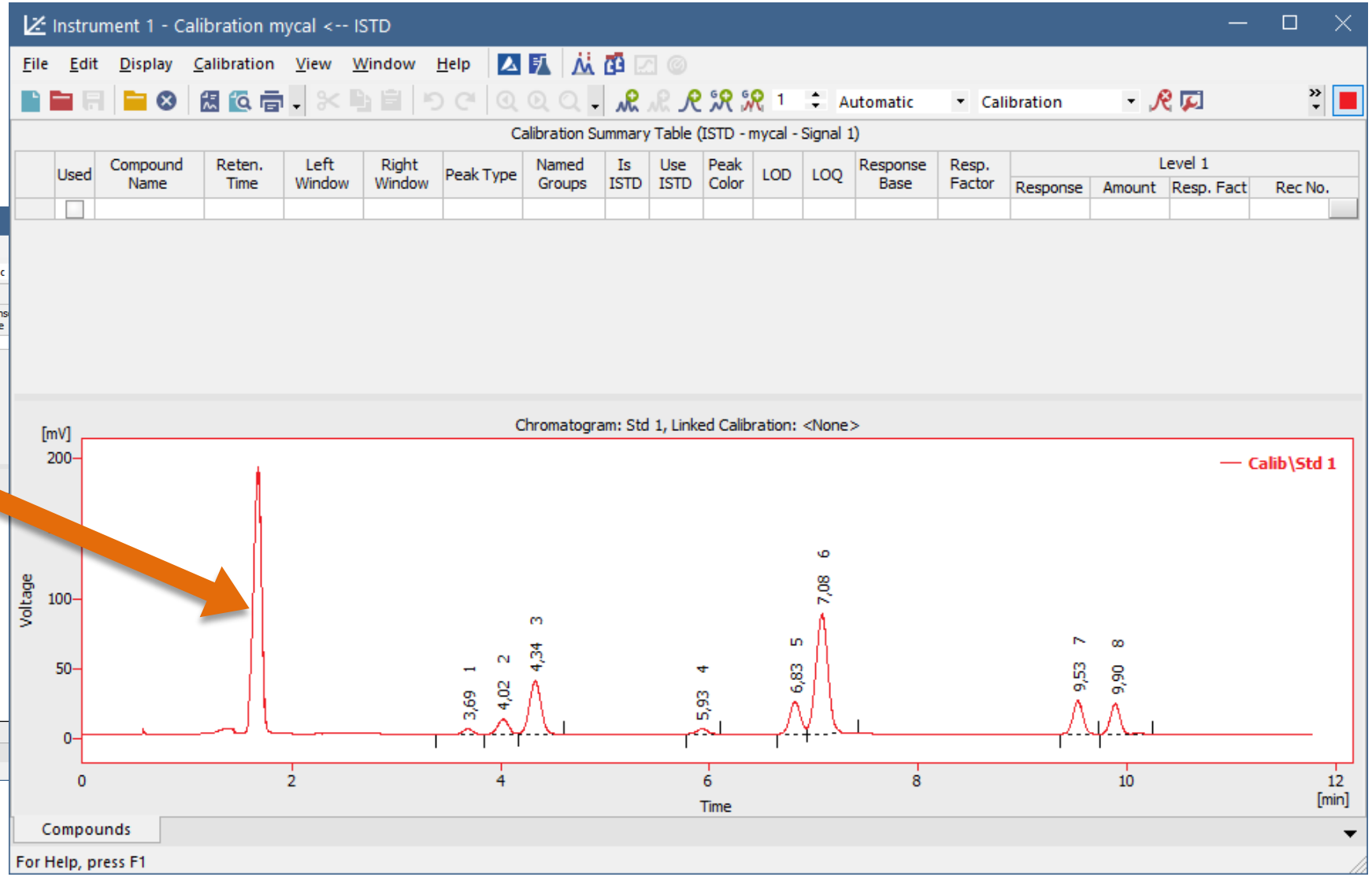


- Calibration
  - Automatic – add all peaks at once
  - Manual – necessary to add peaks one by one
- Units – units‘ name for result tables
- Display Mode – ESTD/ISTD
  - Related to a proper selection calculations
- Mode
  - Automatic – add new levels
  - Recalibrate – for recalibrating selected level

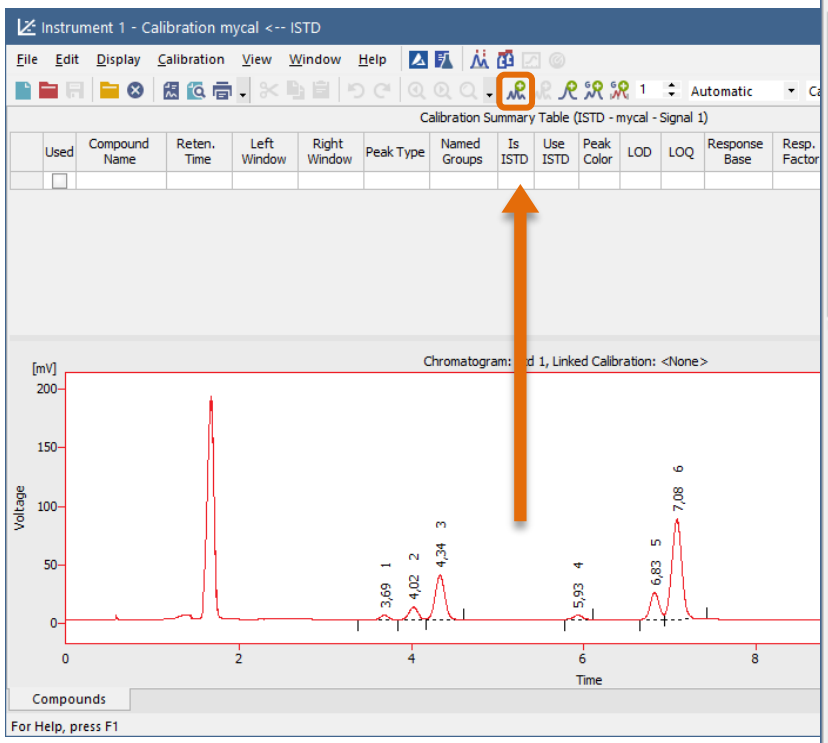


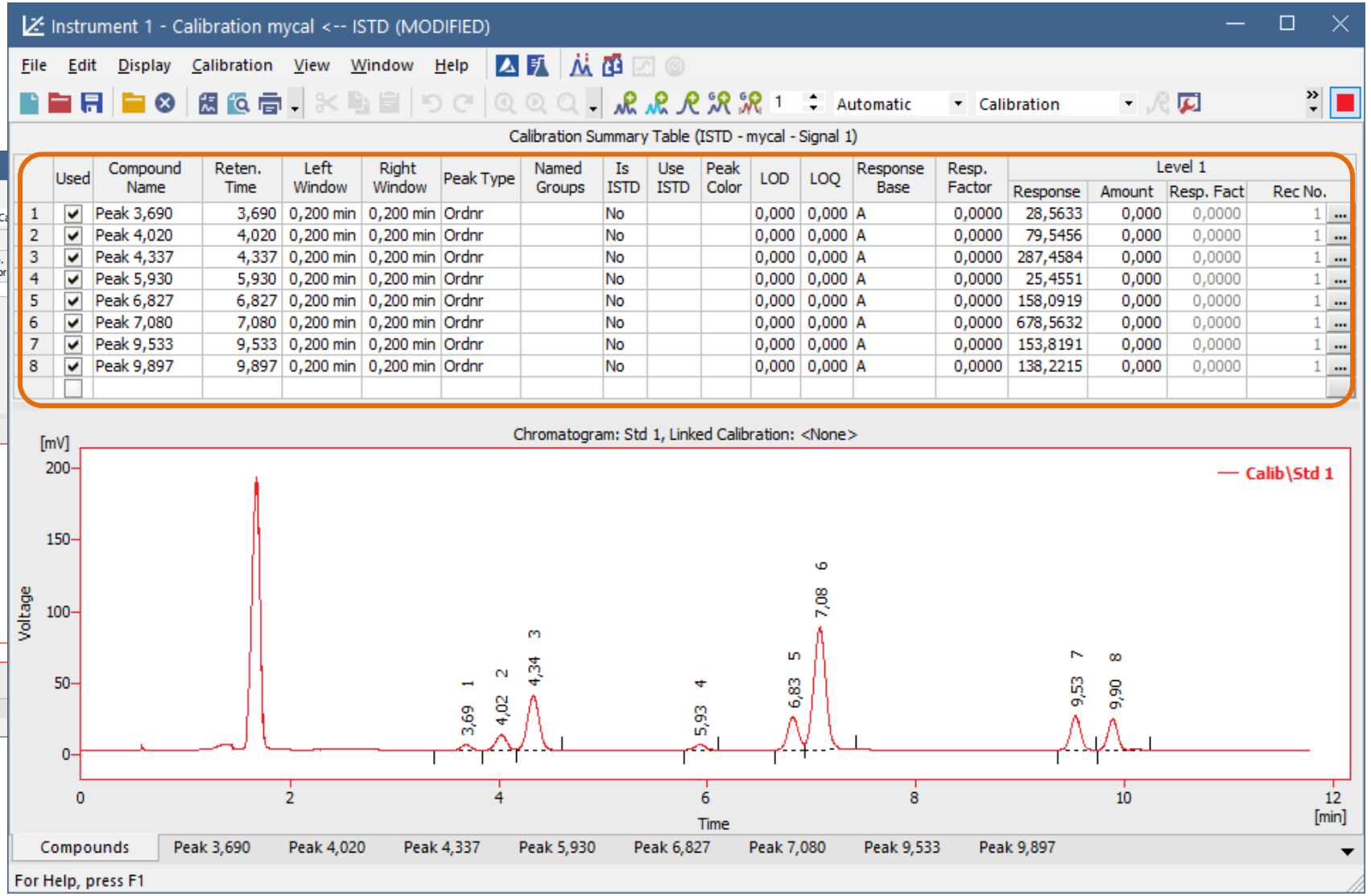
# Open chromatogram of a standard



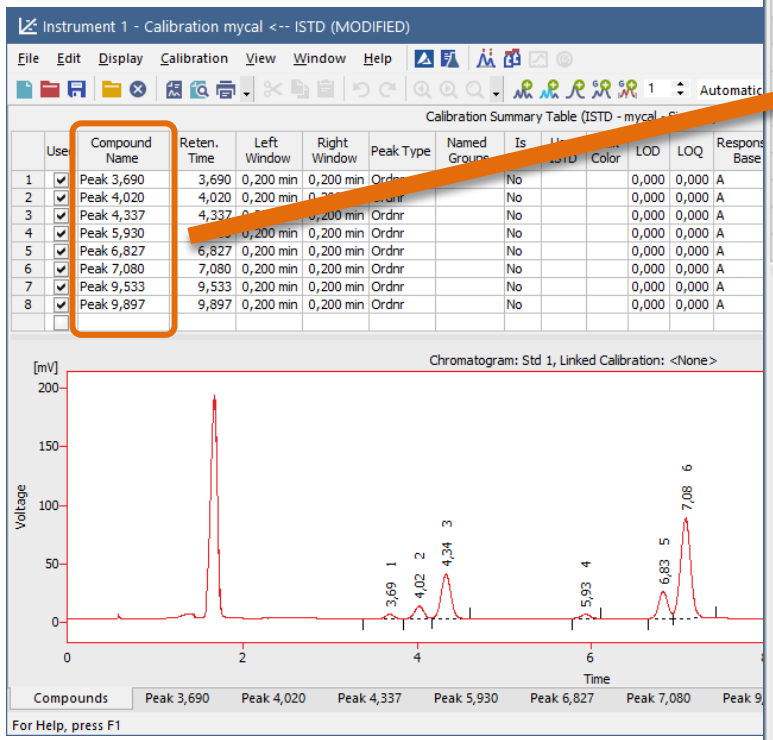



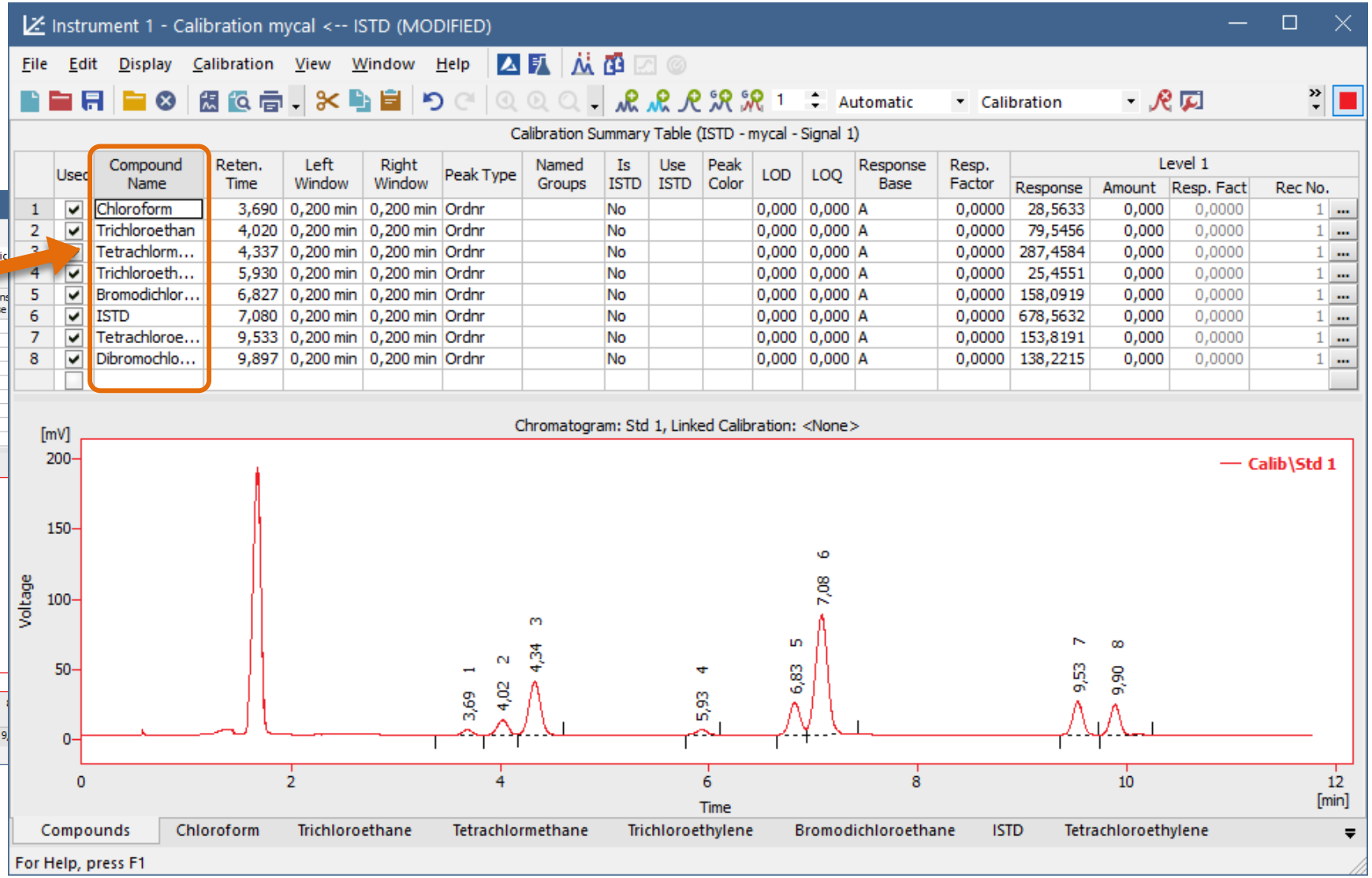
# Add peaks chromatogram to Calibration Summary Table



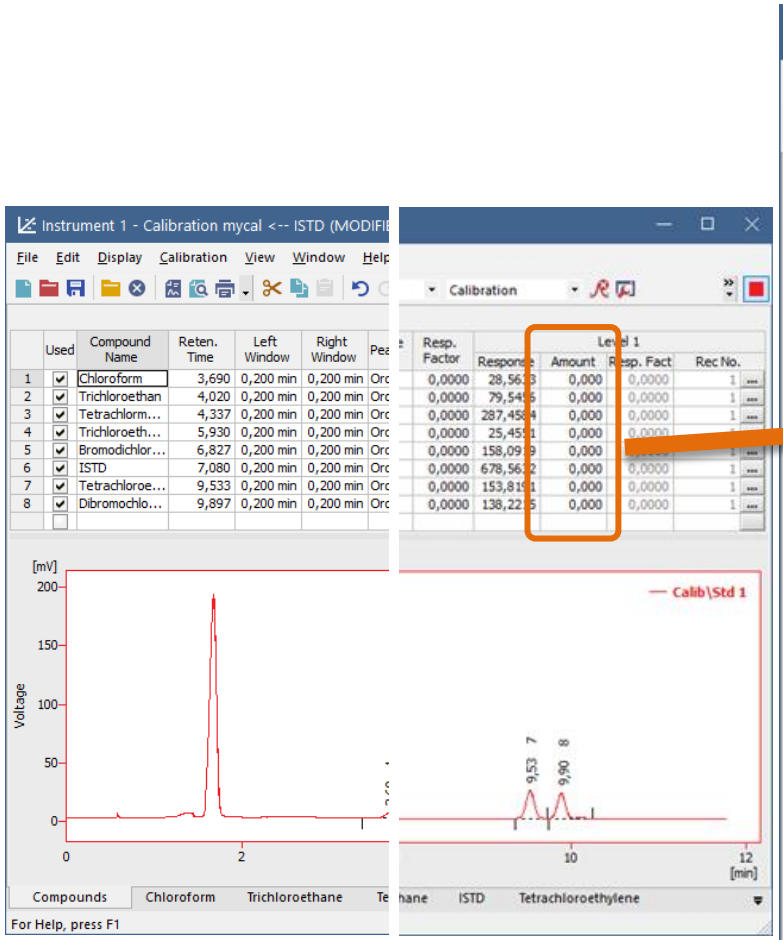



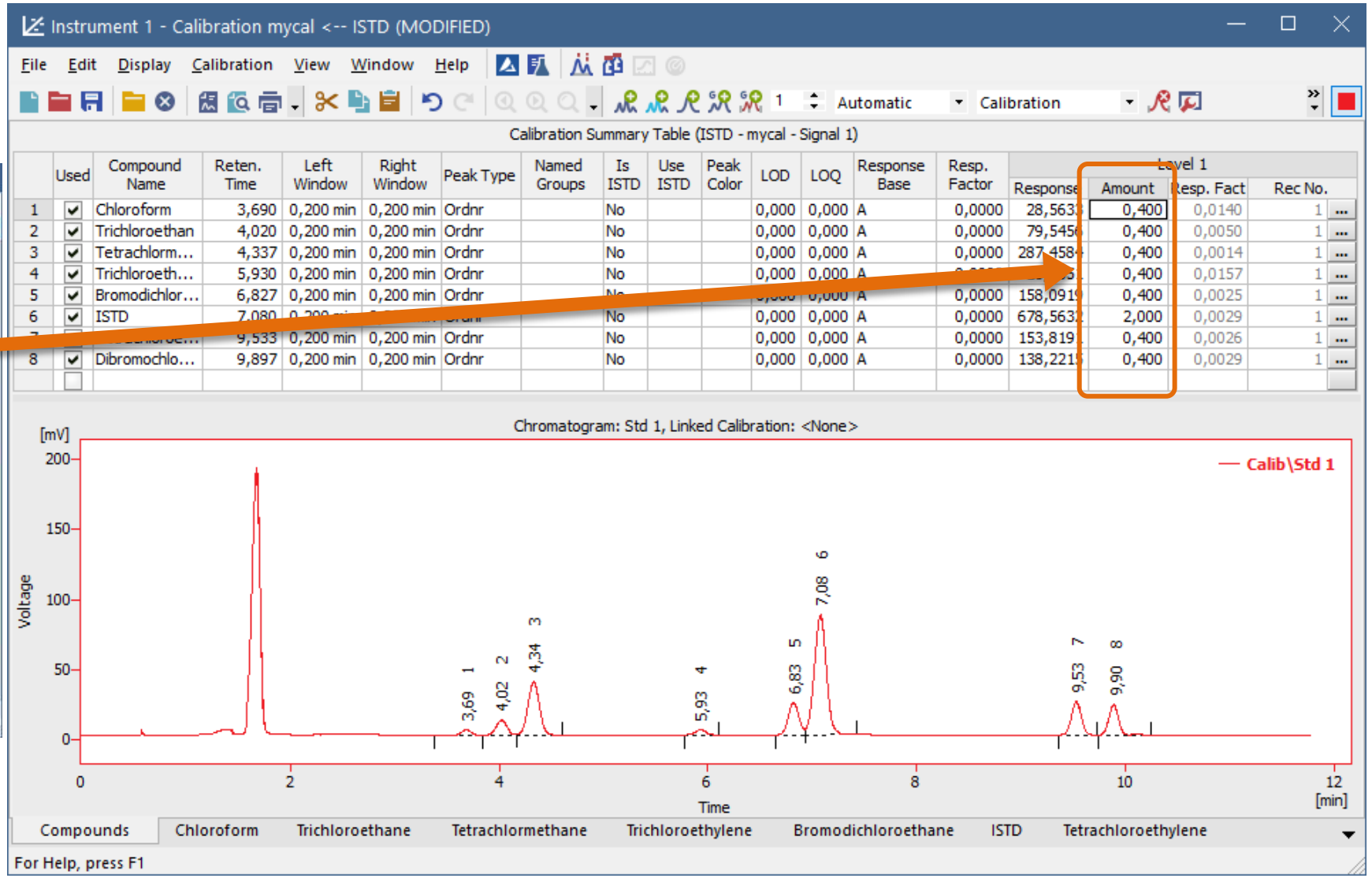
# Edit generic names of compounds (necessary once only)



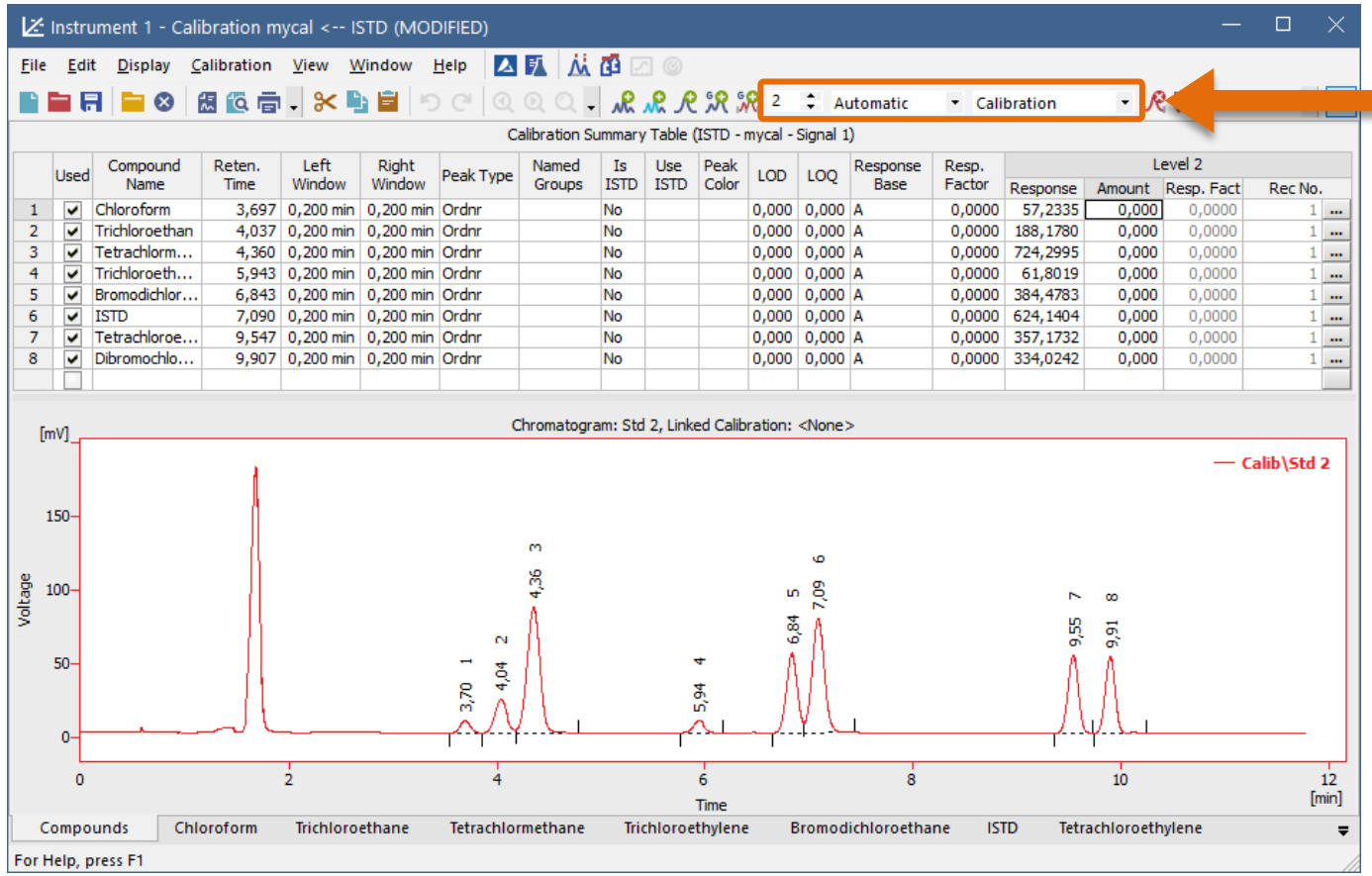



# Enter amounts in Amount column (necessary to repeat for each calibration level)



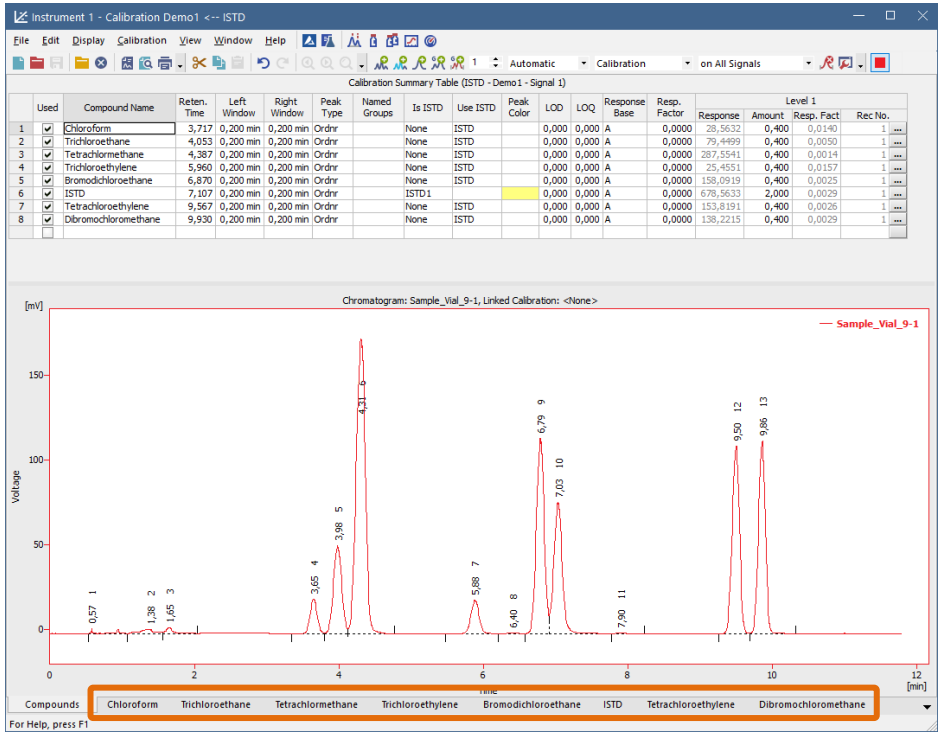



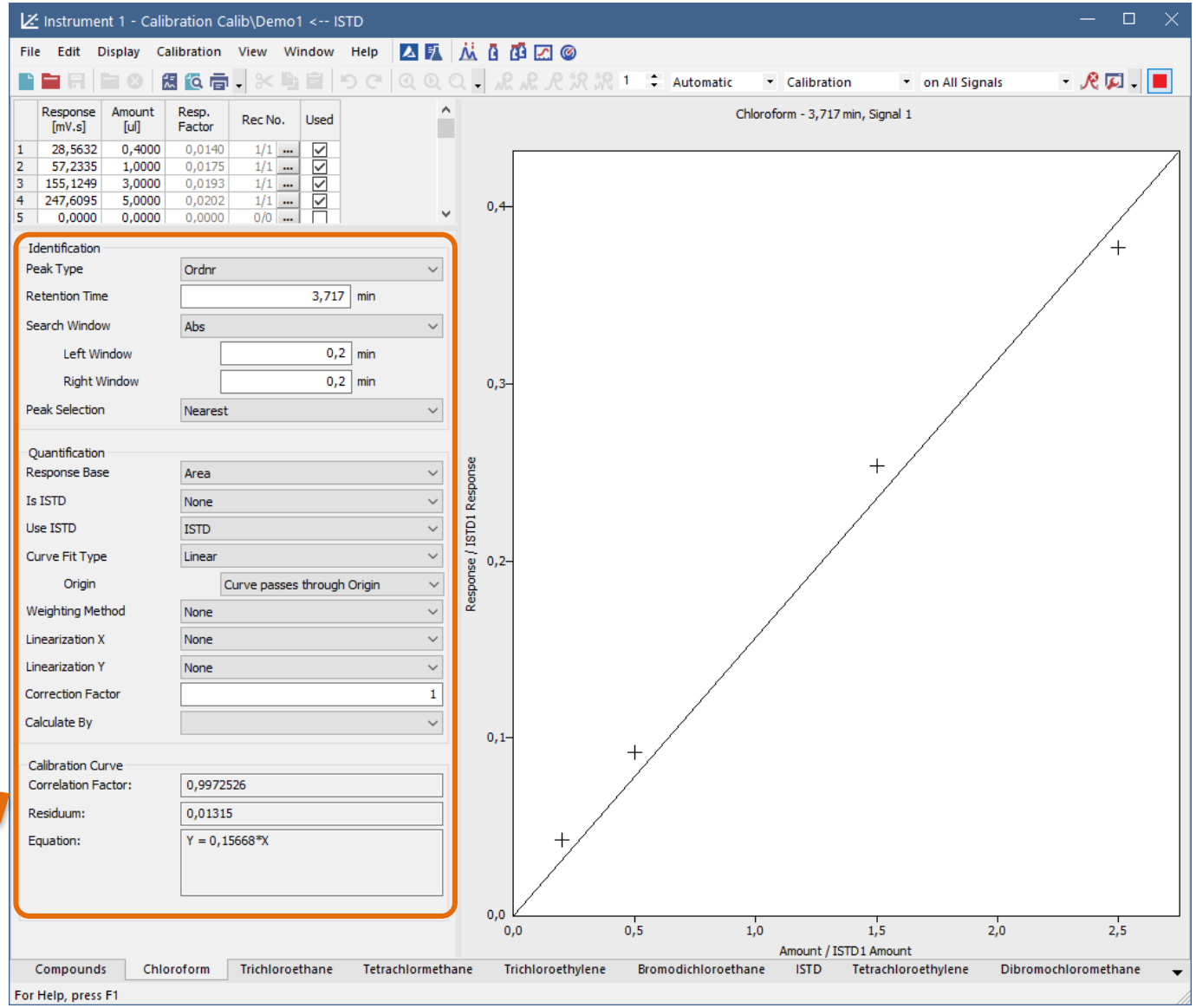
- Repeat this process of adding peaks from standards on multiple levels to build up a multilevel (multipoint) calibration
- Similarly repeat this process on a single level to build up a calibration with replicated/repeated injections of the same standard



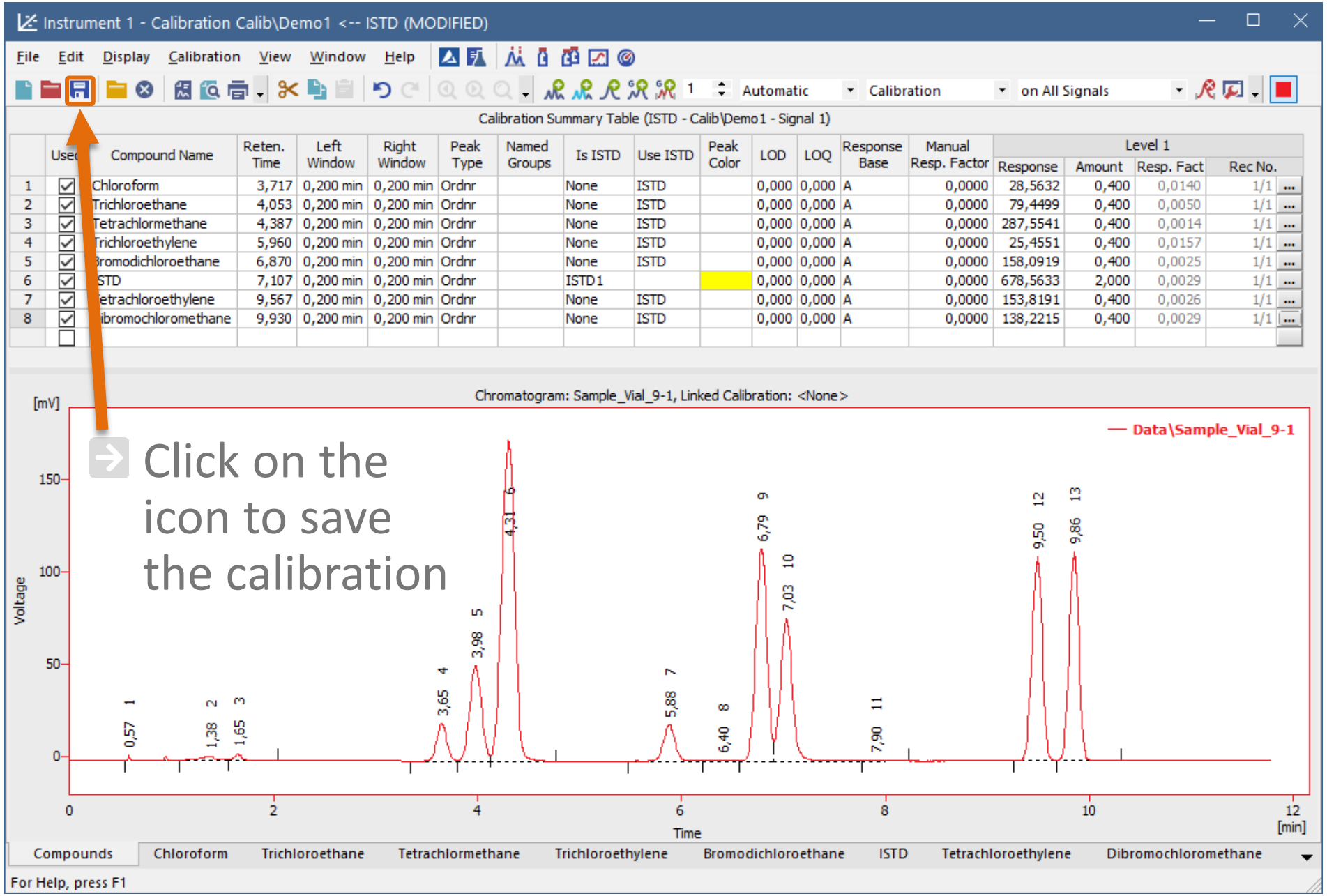

| | Used | Compound Name | Reten. Time | Left Window | Right Window | Peak Type | Named Groups | Is ISTD | Use ISTD | Peak Color | LOD | LOQ | Response Base | Resp. Factor | Level 2 Response | Level 2 Amount | Level 2 Resp. Fact | Level 2 Rec No. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | ✓ | Chloroform | 3,697 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 57,2335 | 0,000 | 0,0000 | 1 |
| 2 | ✓ | Trichloroethan | 4,037 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 188,1780 | 0,000 | 0,0000 | 1 |
| 3 | ✓ | Tetrachlorm… | 4,360 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 724,2995 | 0,000 | 0,0000 | 1 |
| 4 | ✓ | Trichloroeth… | 5,943 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 61,8019 | 0,000 | 0,0000 | 1 |
| 5 | ✓ | Bromodichlor… | 6,843 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 384,4783 | 0,000 | 0,0000 | 1 |
| 6 | ✓ | ISTD | 7,090 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 624,1404 | 0,000 | 0,0000 | 1 |
| 7 | ✓ | Tetrachloroe… | 9,547 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 357,1732 | 0,000 | 0,0000 | 1 |
| 8 | ✓ | Dibromochlo… | 9,907 | 0,200 min | 0,200 min | Ordnr | | No | | | 0,000 | 0,000 | A | 0,0000 | 334,0242 | 0,000 | 0,0000 | 1 |

- With such setting of calibration the peaks will be added to next empty level
- New calibration level is then created this way

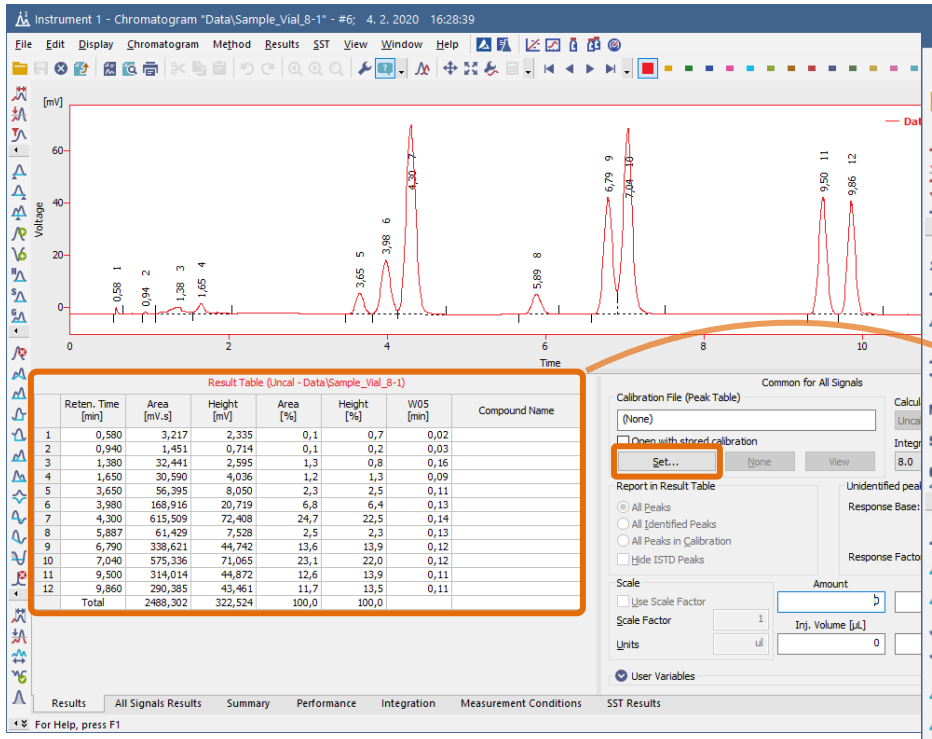


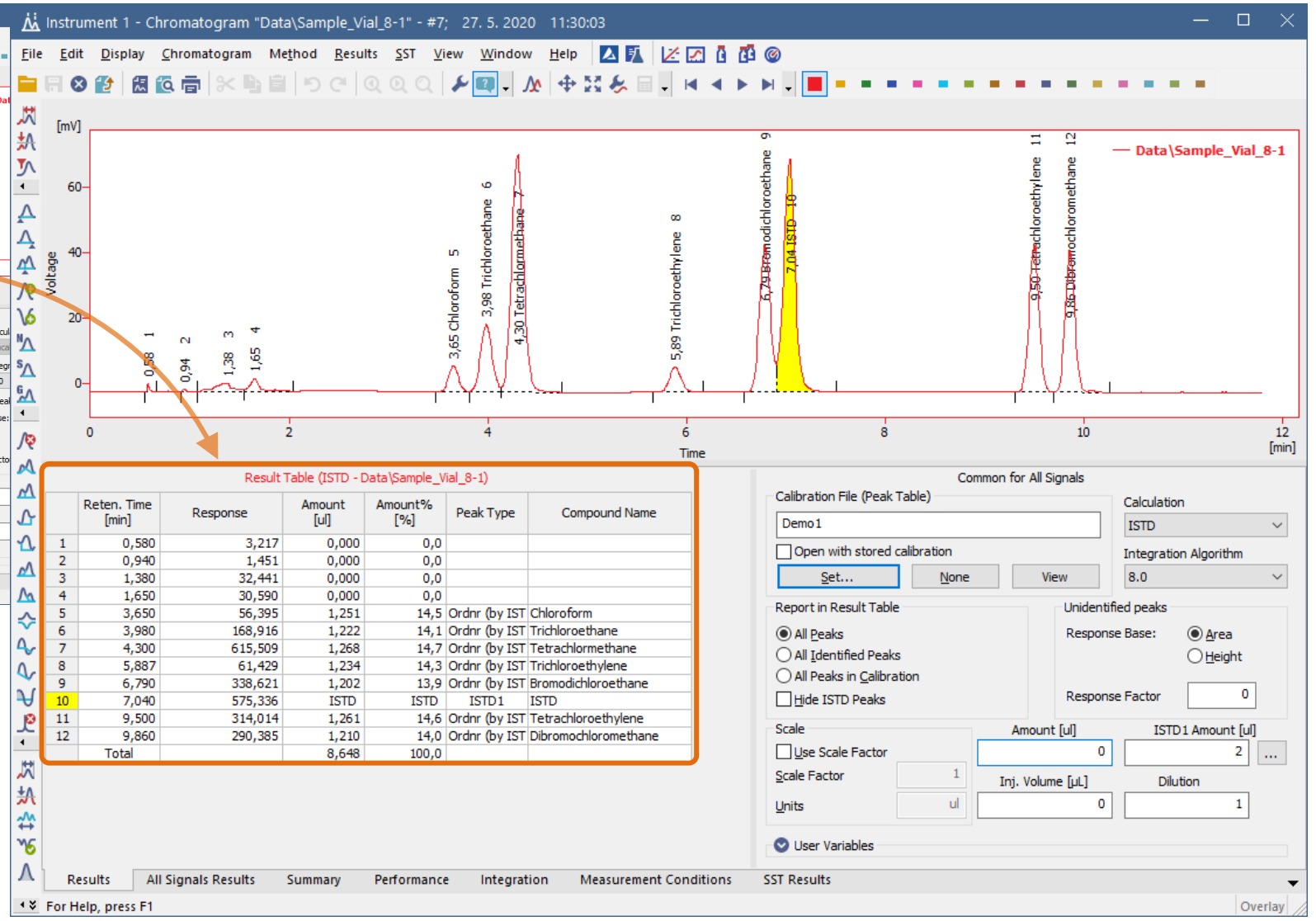




- Click on the tabs to see calibration curve for each compound
- Set options for the calibration curve of individual compound




| | Used | Compound Name | Reten. Time | Left Window | Right Window | Peak Type | Named Groups | Is ISTD | Use ISTD | Peak Color | LOD | LOQ | Response Base | Manual Resp. Factor | Level 1 Response | Level 1 Amount | Level 1 Resp. Fact | Level 1 Rec No. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | ☑ | Chloroform | 3,717 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 28,5632 | 0,400 | 0,0140 | 1/1 |
| 2 | ☑ | Trichloroethane | 4,053 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 79,4499 | 0,400 | 0,0050 | 1/1 |
| 3 | ☑ | Tetrachlormethane | 4,387 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 287,5541 | 0,400 | 0,0014 | 1/1 |
| 4 | ☑ | Trichloroethylene | 5,960 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 25,4551 | 0,400 | 0,0157 | 1/1 |
| 5 | ☑ | Bromodichloroethane | 6,870 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 158,0919 | 0,400 | 0,0025 | 1/1 |
| 6 | ☑ | ISTD | 7,107 | 0,200 min | 0,200 min | Ordnr | | ISTD1 | | | 0,000 | 0,000 | A | 0,0000 | 678,5633 | 2,000 | 0,0029 | 1/1 |
| 7 | ☑ | Tetrachloroethylene | 9,567 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 153,8191 | 0,400 | 0,0026 | 1/1 |
| 8 | ☑ | Dibromochloromethane | 9,930 | 0,200 min | 0,200 min | Ordnr | | None | ISTD | | 0,000 | 0,000 | A | 0,0000 | 138,2215 | 0,400 | 0,0029 | 1/1 |
| | ☐ | | | | | | | | | | | | | | | | | |

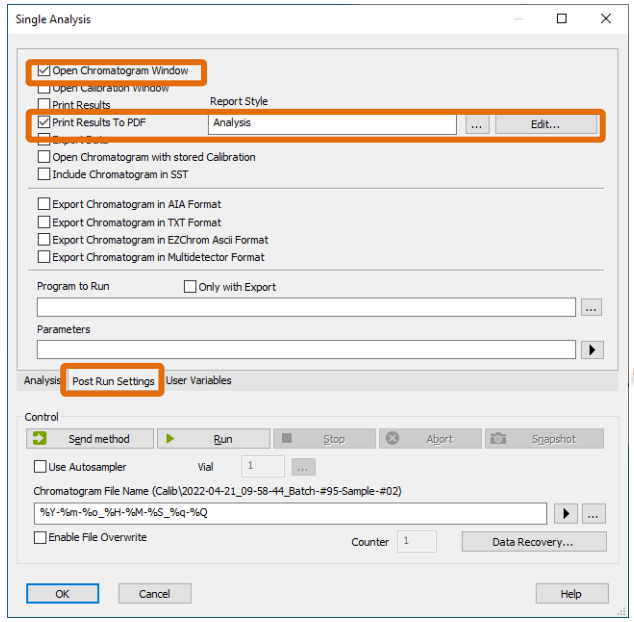


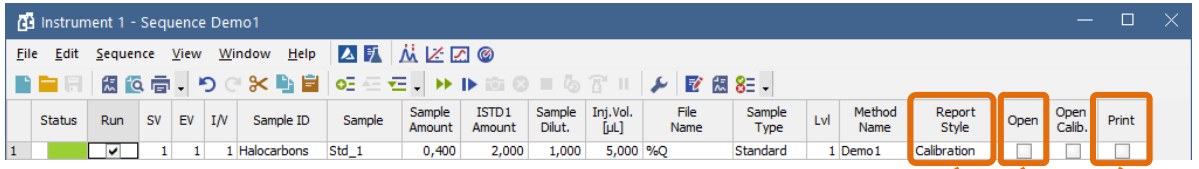



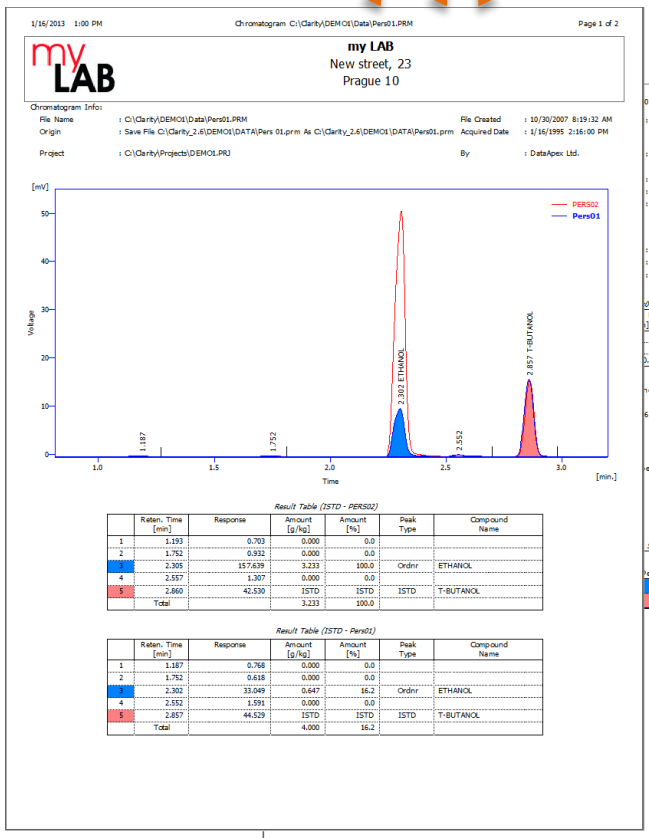

| | Reten. Time [min] | Response | Amount [ul] | Amount% [%] | Peak Type | Compound Name |
|---|---|---|---|---|---|---|
| 1 | 0,580 | 3,217 | 0,000 | 0,0 | | |
| 2 | 0,940 | 1,451 | 0,000 | 0,0 | | |
| 3 | 1,380 | 32,441 | 0,000 | 0,0 | | |
| 4 | 1,650 | 30,590 | 0,000 | 0,0 | | |
| 5 | 3,650 | 56,395 | 1,251 | 14,5 | Ordnr (by IST | Chloroform |
| 6 | 3,980 | 168,916 | 1,222 | 14,1 | Ordnr (by IST | Trichloroethane |
| 7 | 4,300 | 615,509 | 1,268 | 14,7 | Ordnr (by IST | Tetrachlormethane |
| 8 | 5,887 | 61,429 | 1,234 | 14,3 | Ordnr (by IST | Trichloroethylene |
| 9 | 6,790 | 338,621 | 1,202 | 13,9 | Ordnr (by IST | Bromodichloroethane |
| 10 | 7,040 | 575,336 | ISTD | ISTD | ISTD1 | ISTD |
| 11 | 9,500 | 314,014 | 1,261 | 14,6 | Ordnr (by IST | Tetrachloroethylene |
| 12 | 9,860 | 290,385 | 1,210 | 14,0 | Ordnr (by IST | Dibromochloromethane |
| | Total | | 8,648 | 100,0 | | |

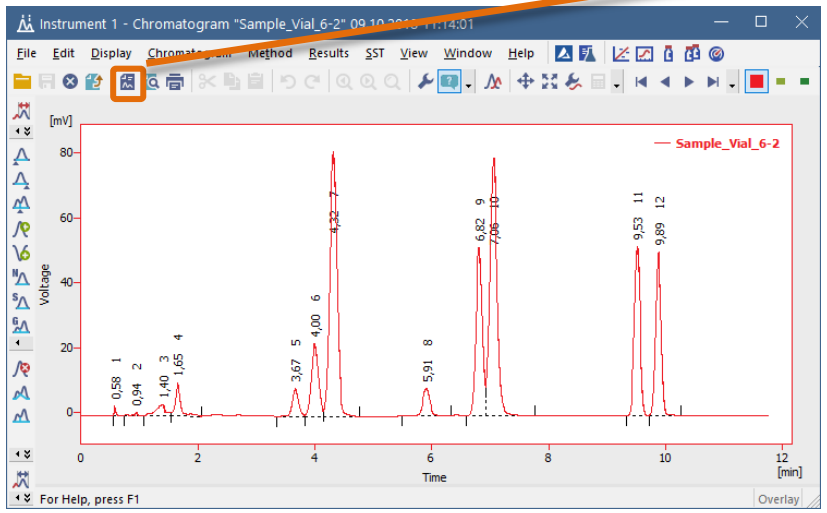
- Select a calibration file to link to the chromatogram
- The compounds will be identified and their amounts in sample will be calculated
- The calibration should be preferably linked in a Method that was used for acquisition of the chromatogram

# Analysis report

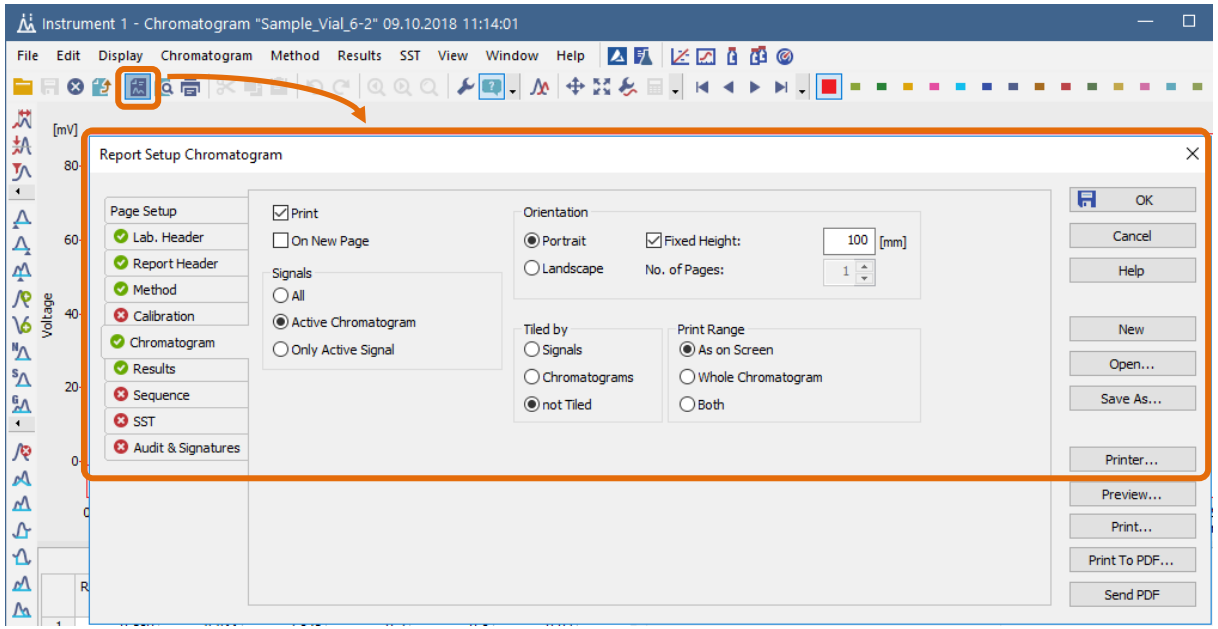


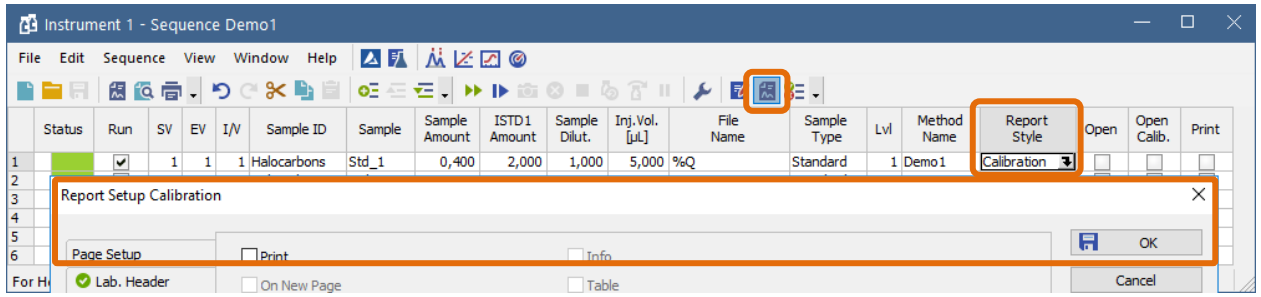



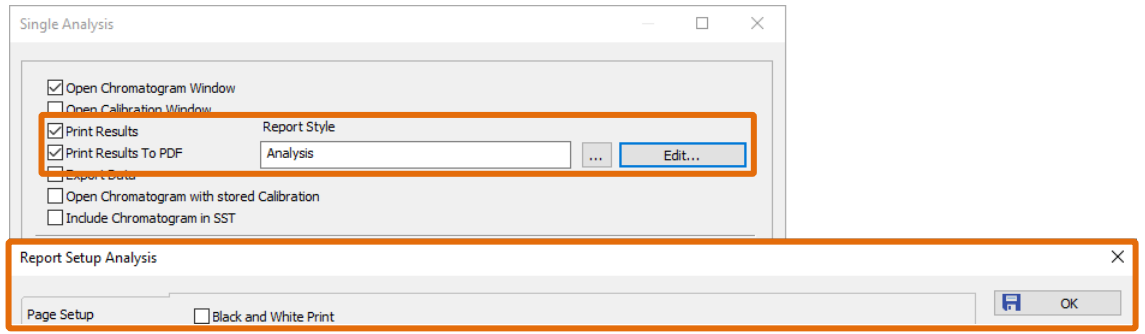



# Analysis report




- Each window (Chromatogram, Calibration etc.) has its own specific setup and contents in the Report
- Report style can be saved as .sty file (COMMON folder)



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# ...THANK YOU FOR YOUR TIME

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