DataApex

SMART SOLUTION FOR LABORATORIES

Clarity™

advanced chromatography software

USER TRAINING

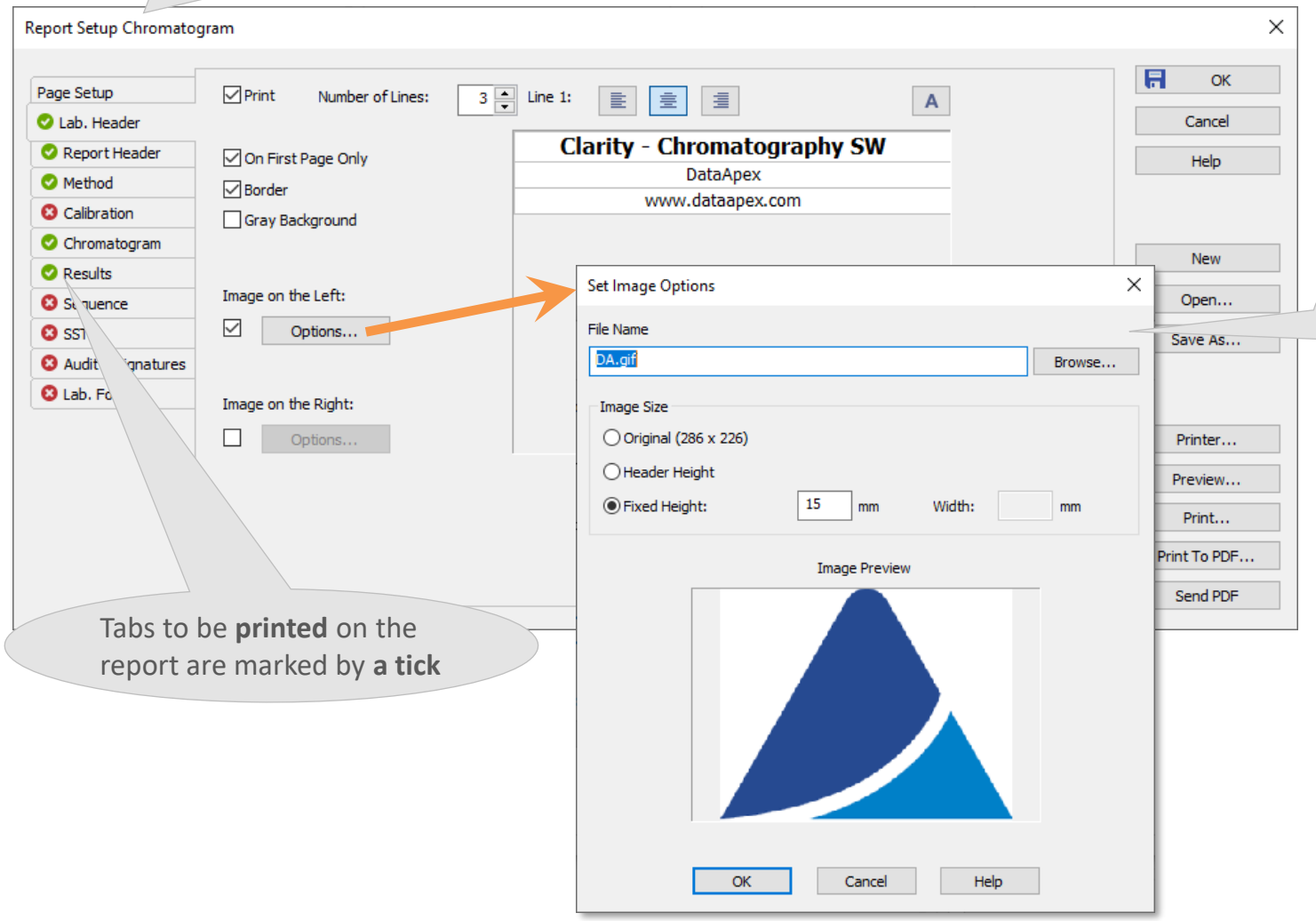
ADVANCED – PART 3

P008/80D 10/2022

Agenda

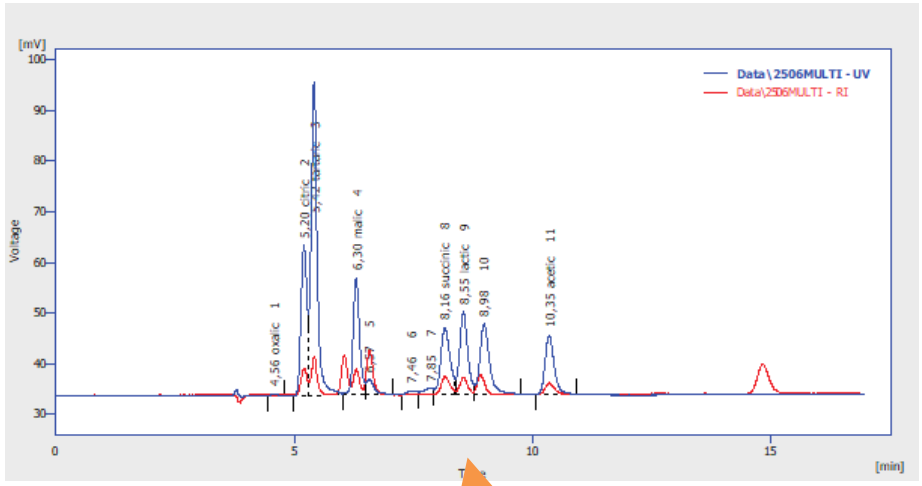
- Reports
  - General, logo and order of sections
- Export Data
  - Number of different ways
  - Chromatogram window
  - Instrument window
- Batch Processing
- Archive & Backup
- Tips & Tricks
  - Perform postrun
  - Customizing toolbars
  - Command lock
  - Most popular shortcuts

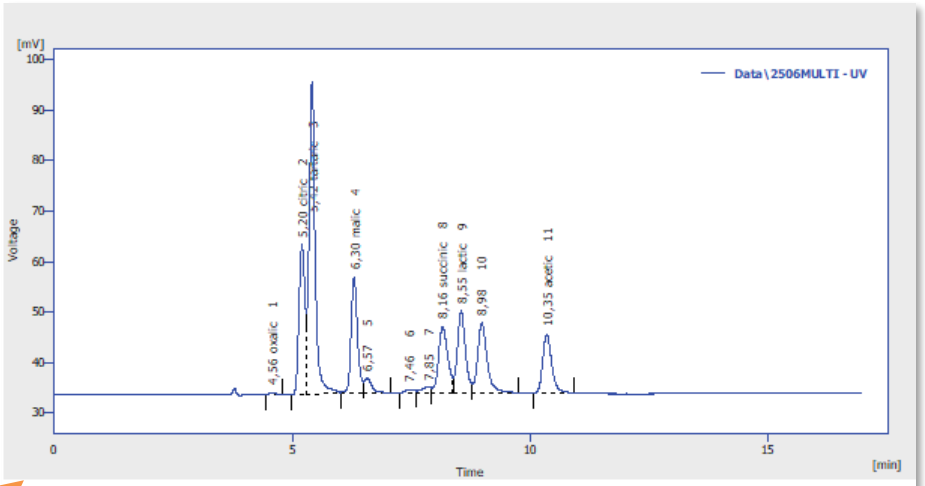
Name of current **Report Style** for the window it was **opened from**

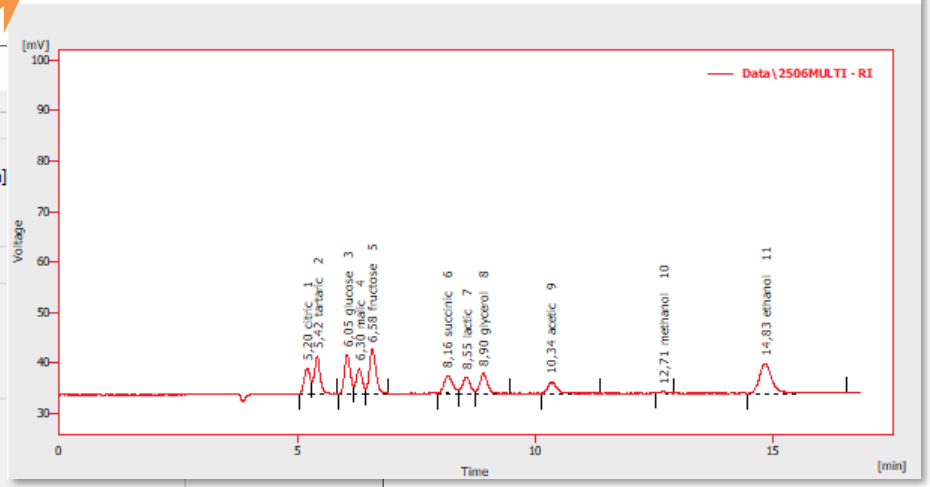


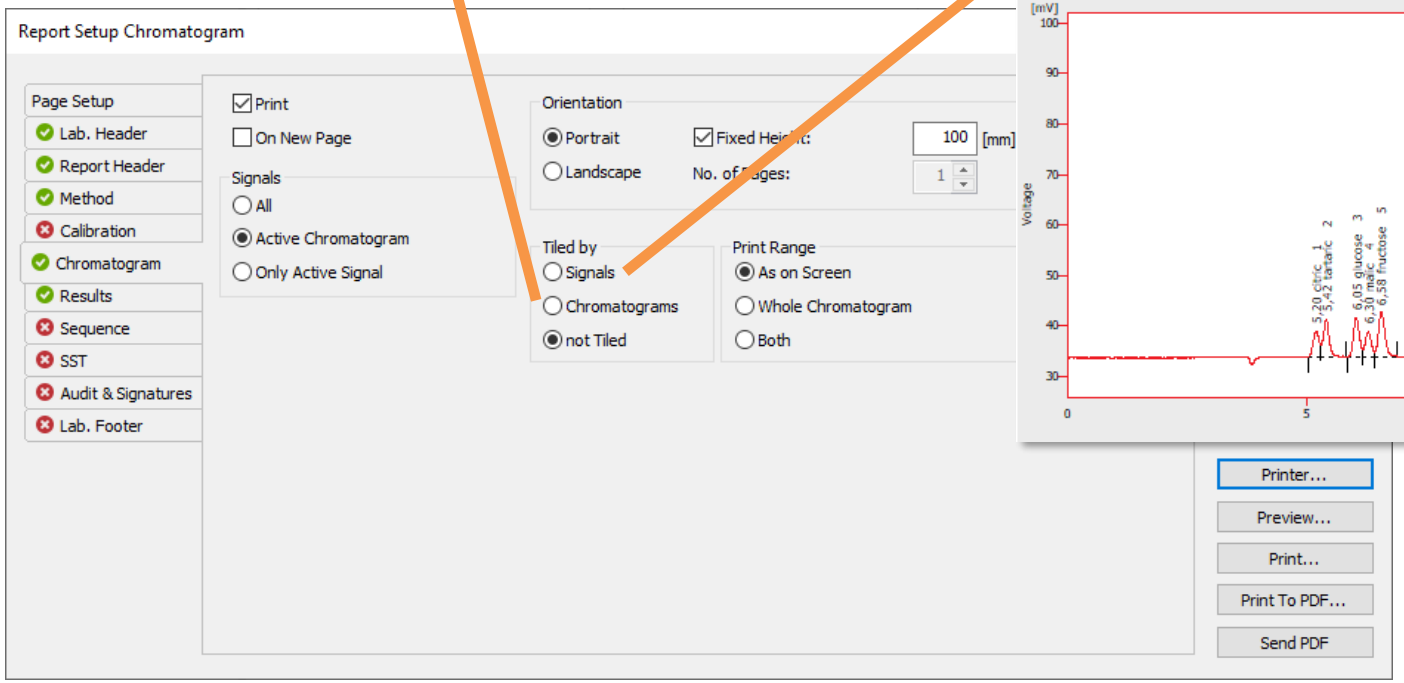
Custom logo in the **Lab. header** of the report

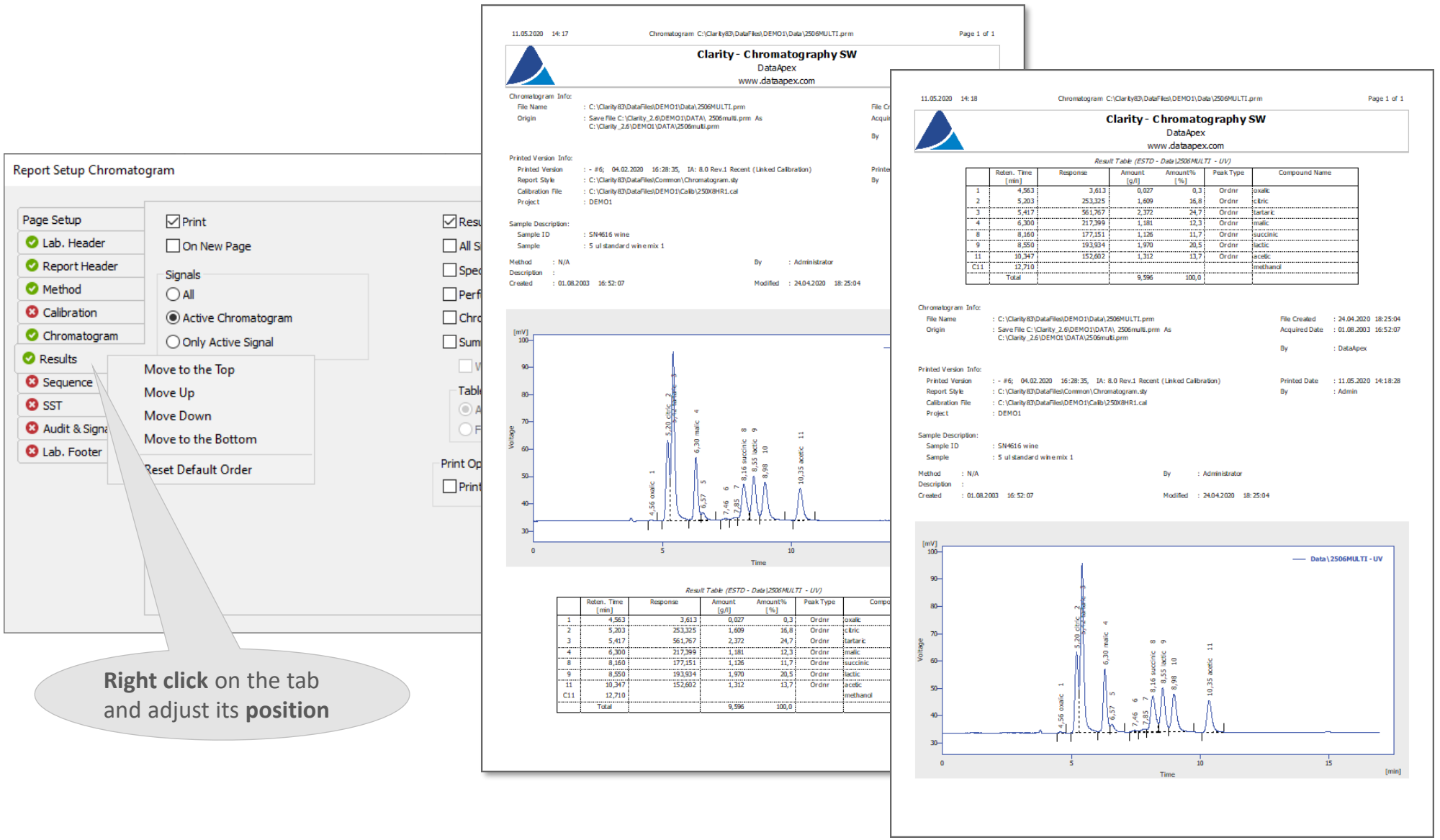
Tabs to be **printed** on the report are marked by **a tick**


[mV]
Data\2506MULTI - UV
Data\2506MULTI - RI
Voltage
4,56 oxalic 1
5,20 citric 2
5,42 tartaric 3
6,30 malic 4
6,57 5
7,46 6
7,85 7
8,16 succinic 8
8,55 lactic 9
8,98 10
10,35 acetic 11
[min]


[mV]
Data\2506MULTI - UV
Voltage
4,56 oxalic 1
5,20 citric 2
5,42 tartaric 3
6,30 malic 4
6,57 5
7,46 6
7,85 7
8,16 succinic 8
8,55 lactic 9
8,98 10
10,35 acetic 11
Time
[min]


[mV]
Data\2506MULTI - RI
Voltage
5,20 citric 1
5,42 tartaric 2
6,05 glucose 3
6,30 malic 4
6,58 fructose 5
8,16 succinic 6
8,55 lactic 7
8,90 glycerol 8
10,34 acetic 9
12,71 methanol 10
14,83 ethanol 11
Time
[min]


Report Setup Chromatogram
Page Setup
Lab. Header
Report Header
Method
Calibration
Chromatogram
Results
Sequence
SST
Audit & Signatures
Lab. Footer
Print
On New Page
Signals
All
Active Chromatogram
Only Active Signal
Orientation
Portrait
Landscape
Fixed Height:
100
[mm]
No. of Pages:
1
Tiled by
Signals
Chromatograms
not Tiled
Print Range
As on Screen
Whole Chromatogram
Both
Printer...
Preview...
Print...
Print To PDF...
Send PDF


Report Setup Chromatogram
Page Setup
Lab. Header
Report Header
Method
Calibration
Chromatogram
Results
Sequence
SST
Audit & Signa
Lab. Footer
Print
On New Page
Signals
All
Active Chromatogram
Only Active Signal
Move to the Top
Move Up
Move Down
Move to the Bottom
Reset Default Order
Right click on the tab and adjust its position
Clarity - Chromatography SW
DataApex
www.dataapex.com
Result Table (ESTD - Data\2506MULTI - UV)
Data\2506MULTI - UV

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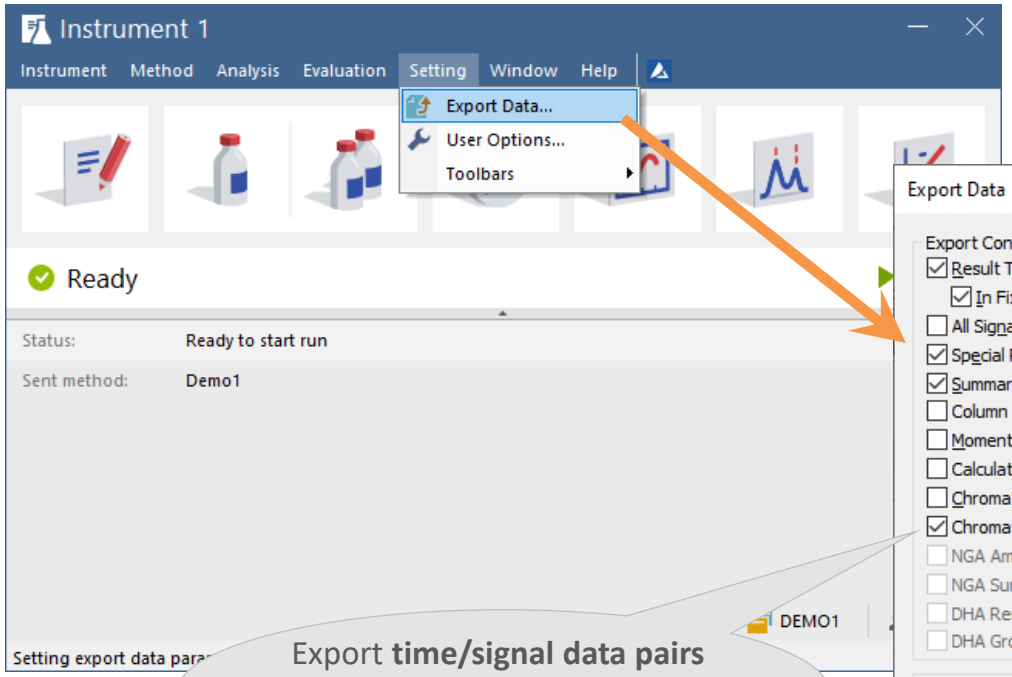
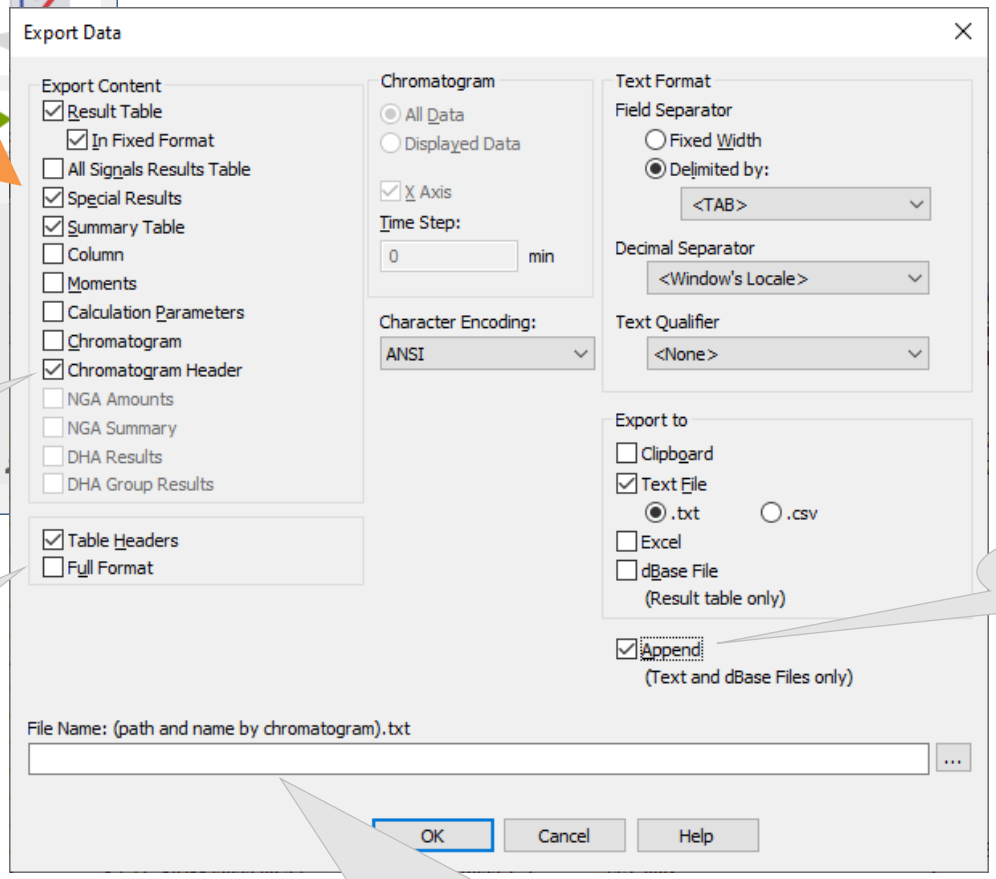
Export data

- **Export data** to other programs for **further processing**
  - Simple **Copy** and **Paste** (Ctrl C – Ctrl V)
- Export Data **settings common** for
  - **manual export** from chromatogram window
  - automatic export from postrun at the **end of each run**
  - automatic export by **batch reprocess** of chromatograms or sequence
- Export of chromatograms in **common formats**

EXPORT DATA → INSTRUMENT WINDOW





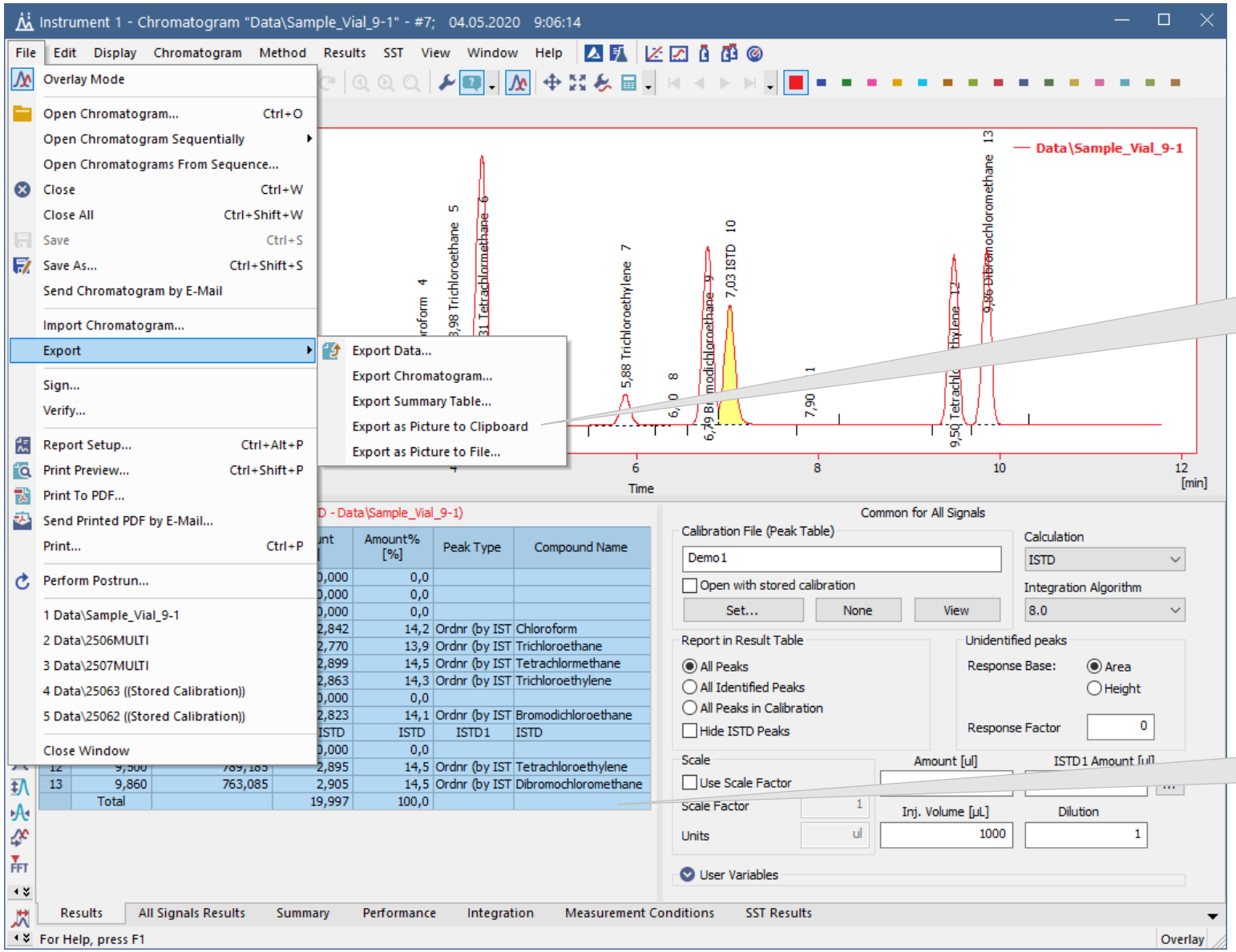
Export **time/signal data pairs** (import to other programs – for example graphics)

Headers: Column headers and chromatogram info
Full format: Filename, date and time before each row

Exports are carried out **into a single file**

blank field = actual chromatogram name + .txt extension
Path can be used also

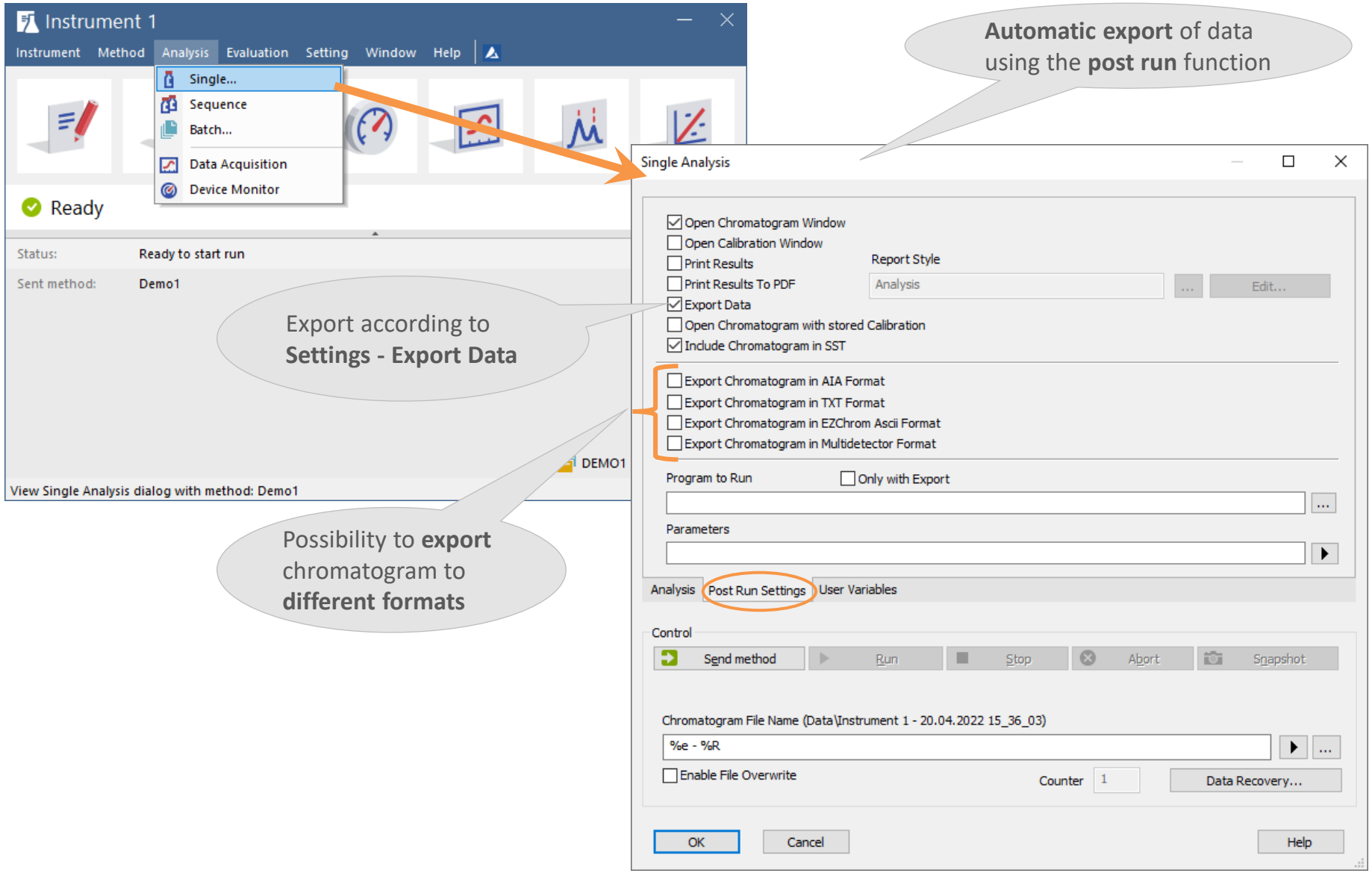
EXPORT DATA → CHROMATOGRAM WINDOW

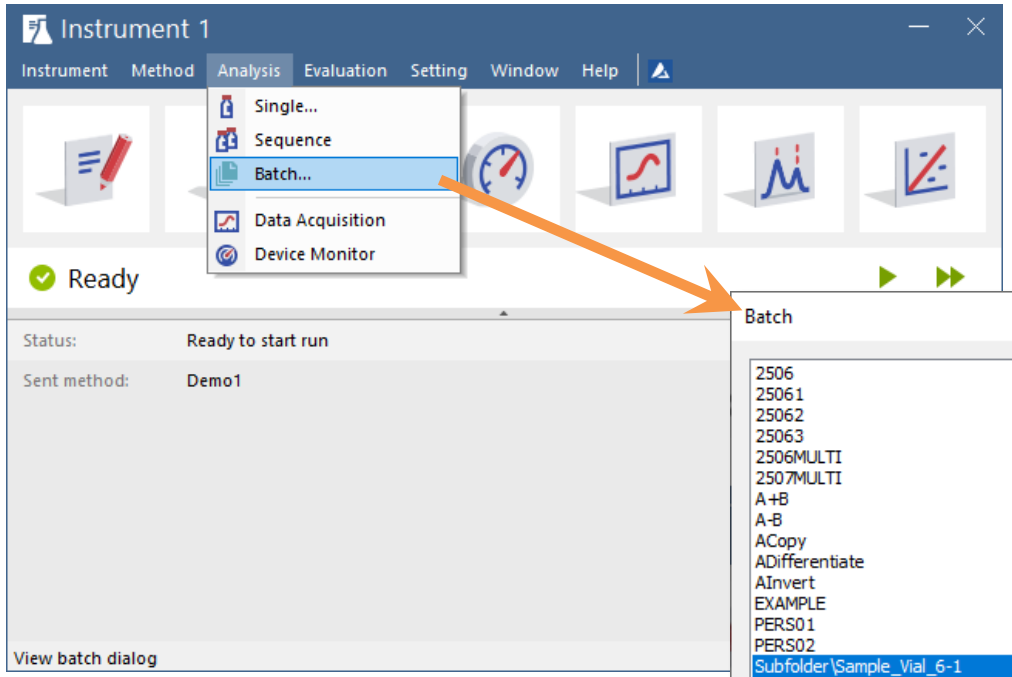


Copy a picture to MS Office (including labels) via **Clipboard or store it in *.emf** format

Select a **part of the result table** and copy it using **Copy** (Ctrl+C) and **Paste** (Ctrl+V)

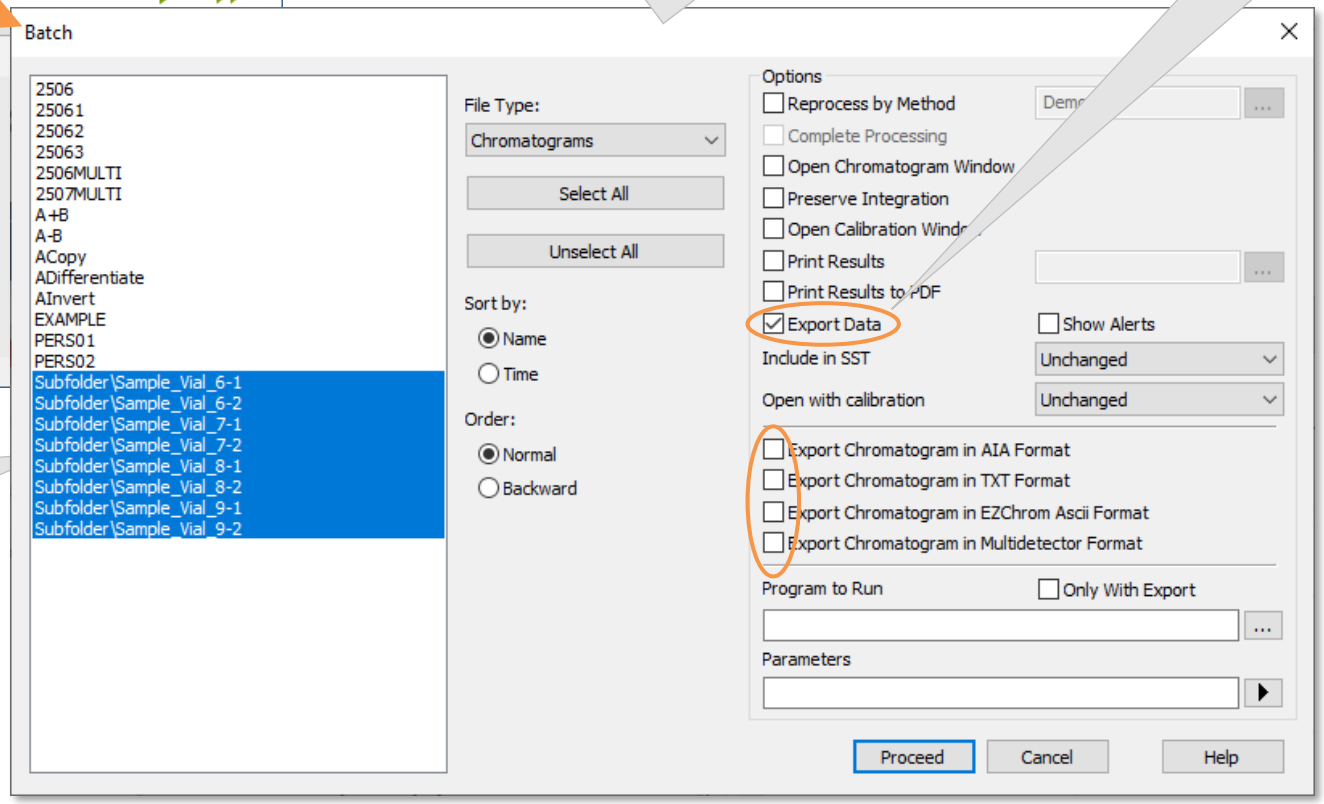
EXPORT DATA → SINGLE ANALYSIS (POST RUN SETTINGS TAB)





Automatically export data from **multiple chromatograms** using the Batch dialog

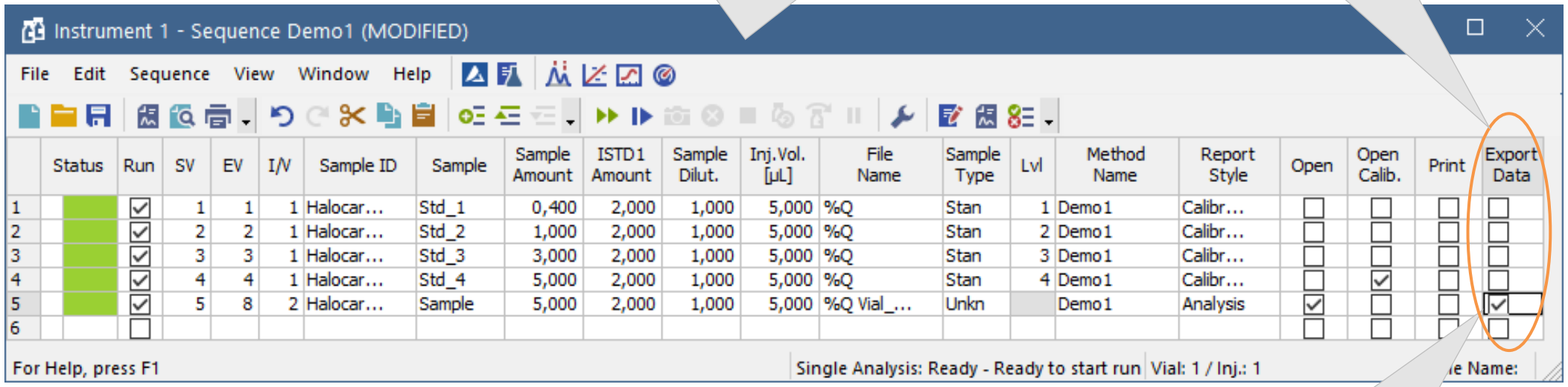
Export according to **Settings - Export Data**



Subfolders are supported in the batch dialog

Automatically export data from the **sequence** table **after** the row has been **measured**

Right mouse click in the table – **Setup columns - Show Export Data**

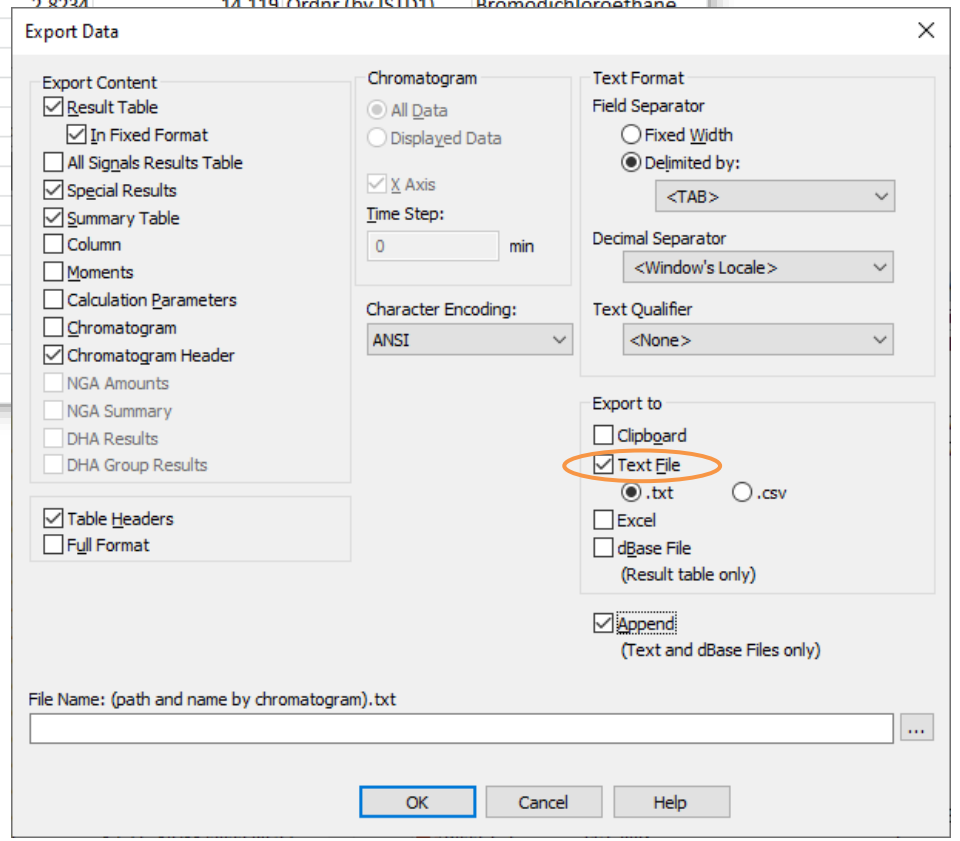


	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print	Export Data
1		☑	1	1	1	Halocar…	Std_1	0,400	2,000	1,000	5,000	%Q	Stan	1	Demo1	Calibr…	☐	☐	☐	☐
2		☑	2	2	1	Halocar…	Std_2	1,000	2,000	1,000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

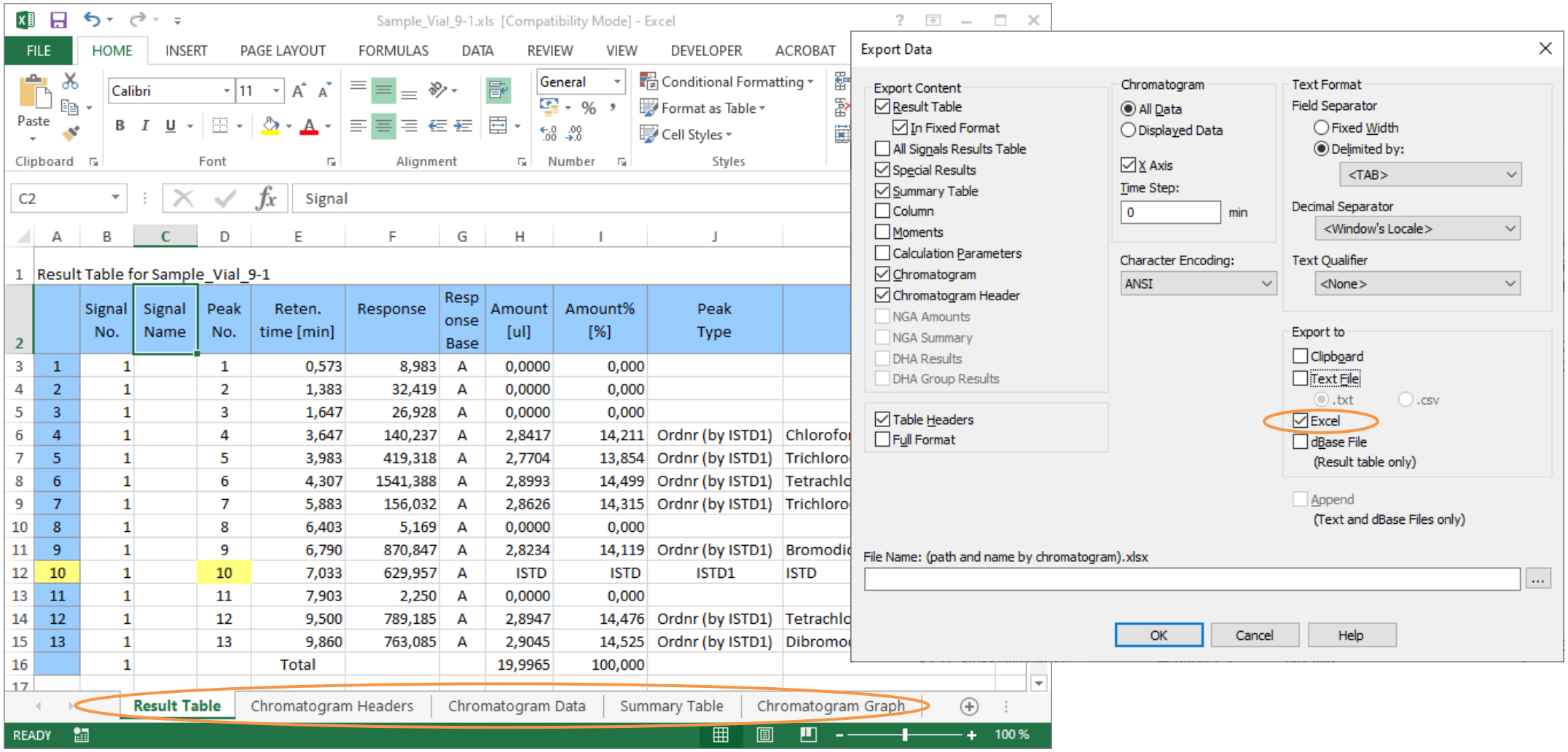
Export according to **Settings - Export Data**

EXPORT DATA → TEXT FILE FORMAT

	1	2	3	4	5	6	7	8	9	10
1	Signal	Signal	Peak	Reten.	Response	Response	Amount	Amount	Peak	Compound
2	No.	Name	No.	time		Base	[ul]	[%]	Type	Name
3	1		1	0,573	8,983	A	0	0		
4	1		2	1,383	32,419	A	0	0		
5	1		3	1,647	26,928	A	0	0		
6	1		4	3,647	140,237	A	2,8417	14,211	Ordnr (by ISTD1)	Chloroform
7	1		5	3,983	419,318	A	2,7704	13,854	Ordnr (by ISTD1)	Trichloroethane
8	1		6	4,307	1541,388	A	2,8993	14,499	Ordnr (by ISTD1)	Tetrachlormethane
9	1		7	5,883	156,032	A	2,8626	14,315	Ordnr (by ISTD1)	Trichloroethylene
10	1		8	6,403	5,169	A	0	0		
11	1		9	6,79	870,847	A	2,8234	14,119	Ordnr (by ISTD1)	Bromodichloroethane
12	1		10	7,033	629,957	A	ISTD			
13	1		11	7,903	2,25	A				
14	1		12	9,5	789,185	A				
15	1		13	9,86	763,085	A				
16	1			Total						
17										
18	Primary file :	Sample_Vial_9-1	Analyst :	Administrator						
19	Sample ID :	Halocarbons	From :	Tue, 03rd Aug, 2004	0:00:00					
20	Sample :	Sample								
21	Instrument :	<Unknown>	Method :	<Unknown>						
22	Sample Amount:	0	ISTD Am. :	2						
23	Sample Dilut.:	1	Inj. Vol.:	1						
24	Peak width :	0,001	Threshold :	0						



EXPORT DATA → EXCEL (*.XLSX) FORMAT



		Signal No.	Signal Name	Peak No.	Reten. time [min]	Response	Response Base	Amount [ul]	Amount% [%]	Peak Type	
3	1	1		1	0,573	8,983	A	0,0000	0,000		
4	2	1		2	1,383	32,419	A	0,0000	0,000		
5	3	1		3	1,647	26,928	A	0,0000	0,000		
6	4	1		4	3,647	140,237	A	2,8417	14,211	Ordnr (by ISTD1)	Chlorofo
7	5	1		5	3,983	419,318	A	2,7704	13,854	Ordnr (by ISTD1)	Trichloro
8	6	1		6	4,307	1541,388	A	2,8993	14,499	Ordnr (by ISTD1)	Tetrachlo
9	7	1		7	5,883	156,032	A	2,8626	14,315	Ordnr (by ISTD1)	Trichloro
10	8	1		8	6,403	5,169	A	0,0000	0,000		
11	9	1		9	6,790	870,847	A	2,8234	14,119	Ordnr (by ISTD1)	Bromodi
12	10	1		10	7,033	629,957	A	ISTD	ISTD	ISTD1	ISTD
13	11	1		11	7,903	2,250	A	0,0000	0,000		
14	12	1		12	9,500	789,185	A	2,8947	14,476	Ordnr (by ISTD1)	Tetrachlo
15	13	1		13	9,860	763,085	A	2,9045	14,525	Ordnr (by ISTD1)	Dibromo
16		1			Total			19,9965	100,000		

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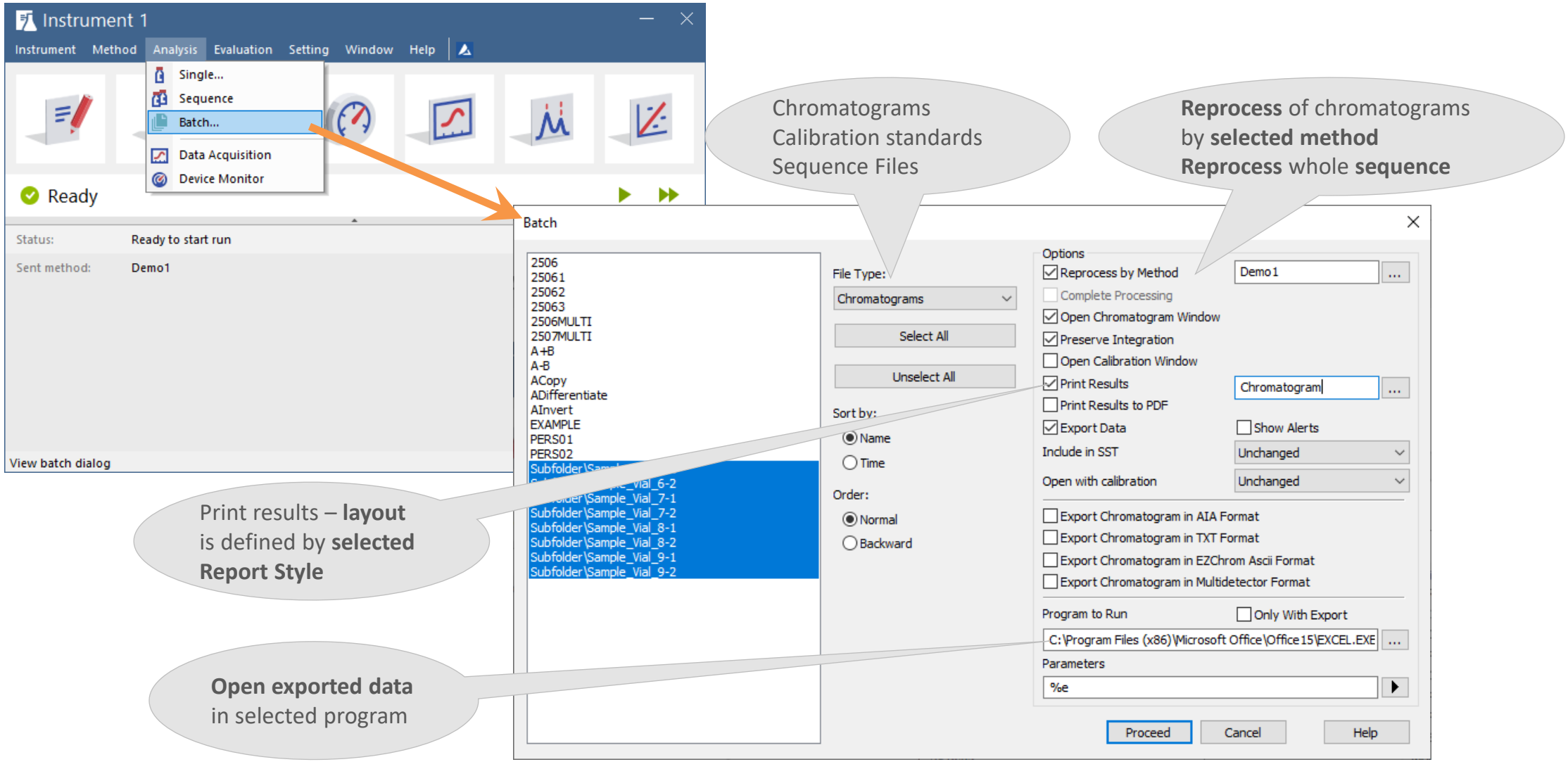
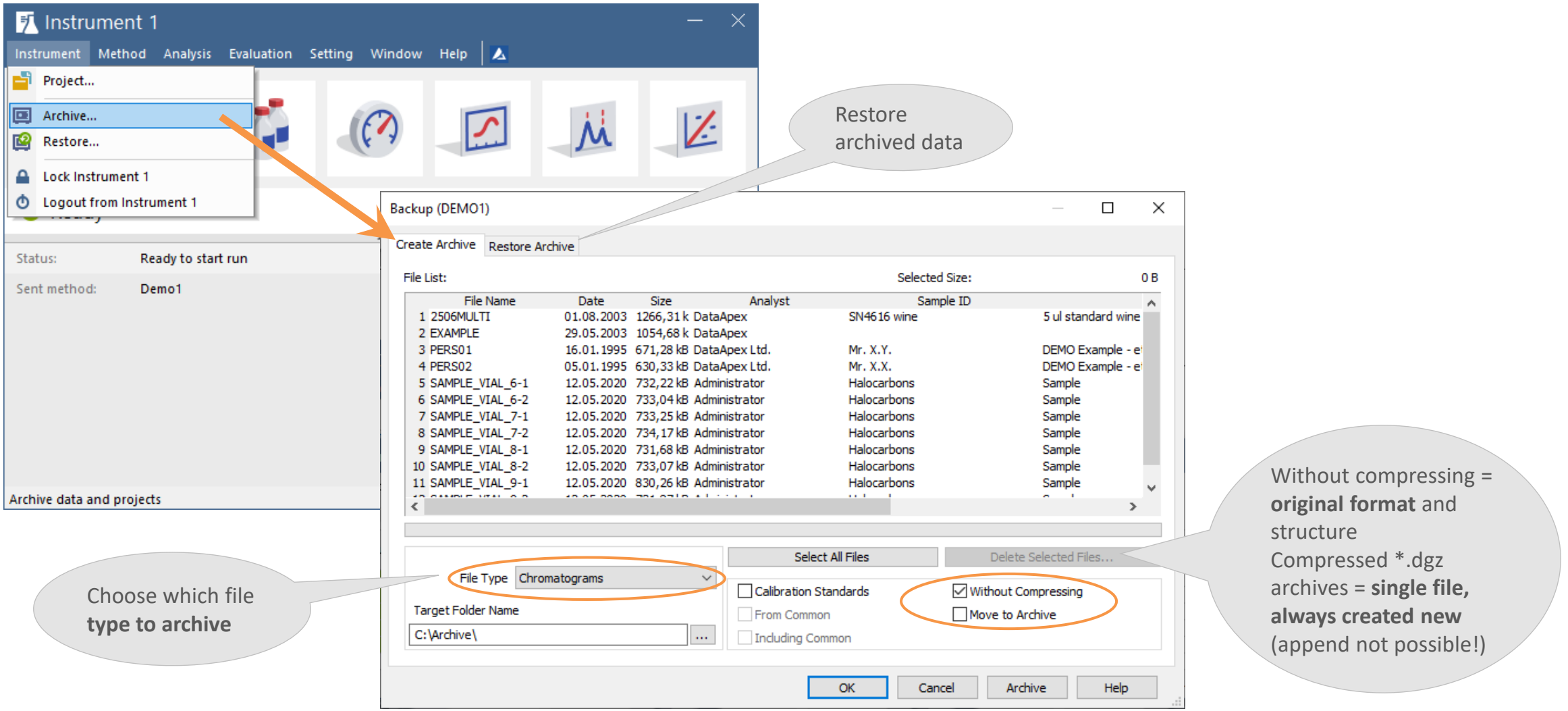

Instrument 1
Instrument
Method
Analysis
Evaluation
Setting
Window
Help
Single...
Sequence
Batch...
Data Acquisition
Device Monitor
Ready
Status:
Ready to start run
Sent method:
Demo1
View batch dialog
Chromatograms
Calibration standards
Sequence Files
Reprocess of chromatograms by selected method
Reprocess whole sequence
Print results – layout is defined by selected Report Style
Open exported data in selected program
Batch
2506
25061
25062
25063
2506MULTI
2507MULTI
A+B
A-B
ACopy
ADifferentiate
AInvert
EXAMPLE
PERS01
PERS02
Subfolder\Sample_Vial_7-1
Subfolder\Sample_Vial_7-2
Subfolder\Sample_Vial_8-1
Subfolder\Sample_Vial_8-2
Subfolder\Sample_Vial_9-1
Subfolder\Sample_Vial_9-2
File Type:
Chromatograms
Select All
Unselect All
Sort by:
Name
Time
Order:
Normal
Backward
Options
Reprocess by Method
Demo1
Complete Processing
Open Chromatogram Window
Preserve Integration
Open Calibration Window
Print Results
Chromatogram
Print Results to PDF
Export Data
Show Alerts
Include in SST
Unchanged
Open with calibration
Unchanged
Export Chromatogram in AIA Format
Export Chromatogram in TXT Format
Export Chromatogram in EZChrom Ascii Format
Export Chromatogram in Multidetector Format
Program to Run
Only With Export
C:\Program Files (x86)\Microsoft Office\Office15\EXCEL.EXE
Parameters
%e
Proceed
Cancel
Help

Overview

- To **reduce** the data **size**, **compressed archive *.dgz** files should be used
- *.dgz archives **always replace all data**
  (files deleted from project will be also deleted from the archive during archiving)
- It is **advantageous** to **archive whole projects**
  - Should be considered when **planning project structure**


Instrument 1
Instrument
Method
Analysis
Evaluation
Setting
Window
Help
Project...
Archive...
Restore...
Lock Instrument 1
Logout from Instrument 1
Status:
Ready to start run
Sent method:
Demo1
Archive data and projects
Restore archived data
Backup (DEMO1)
Create Archive
Restore Archive
File List:
Selected Size:
0 B
File Name
Date
Size
Analyst
Sample ID
1 2506MULTI 01.08.2003 1266,31 k DataApex SN4616 wine 5 ul standard wine
2 EXAMPLE 29.05.2003 1054,68 k DataApex
3 PERS01 16.01.1995 671,28 kB DataApex Ltd. Mr. X.Y. DEMO Example - e
4 PERS02 05.01.1995 630,33 kB DataApex Ltd. Mr. X.X. DEMO Example - e
5 SAMPLE_VIAL_6-1 12.05.2020 732,22 kB Administrator Halocarbons Sample
6 SAMPLE_VIAL_6-2 12.05.2020 733,04 kB Administrator Halocarbons Sample
7 SAMPLE_VIAL_7-1 12.05.2020 733,25 kB Administrator Halocarbons Sample
8 SAMPLE_VIAL_7-2 12.05.2020 734,17 kB Administrator Halocarbons Sample
9 SAMPLE_VIAL_8-1 12.05.2020 731,68 kB Administrator Halocarbons Sample
10 SAMPLE_VIAL_8-2 12.05.2020 733,07 kB Administrator Halocarbons Sample
11 SAMPLE_VIAL_9-1 12.05.2020 830,26 kB Administrator Halocarbons Sample
Select All Files
Delete Selected Files...
File Type
Chromatograms
Target Folder Name
C:\Archive\
Calibration Standards
From Common
Including Common
Without Compressing
Move to Archive
OK
Cancel
Archive
Help
Choose which file type to archive
Without compressing = original format and structure
Compressed *.dgz archives = single file, always created new (append not possible!)

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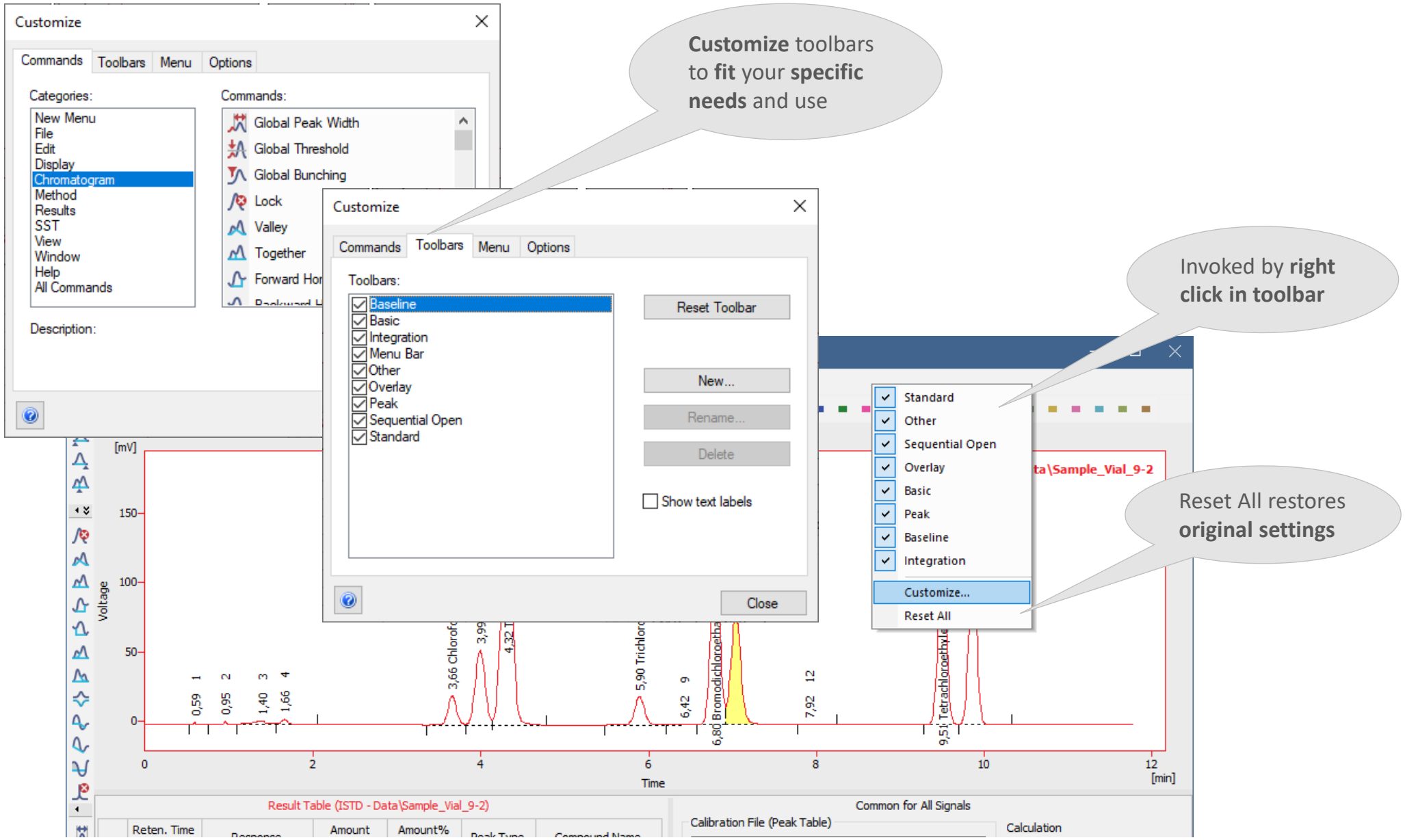
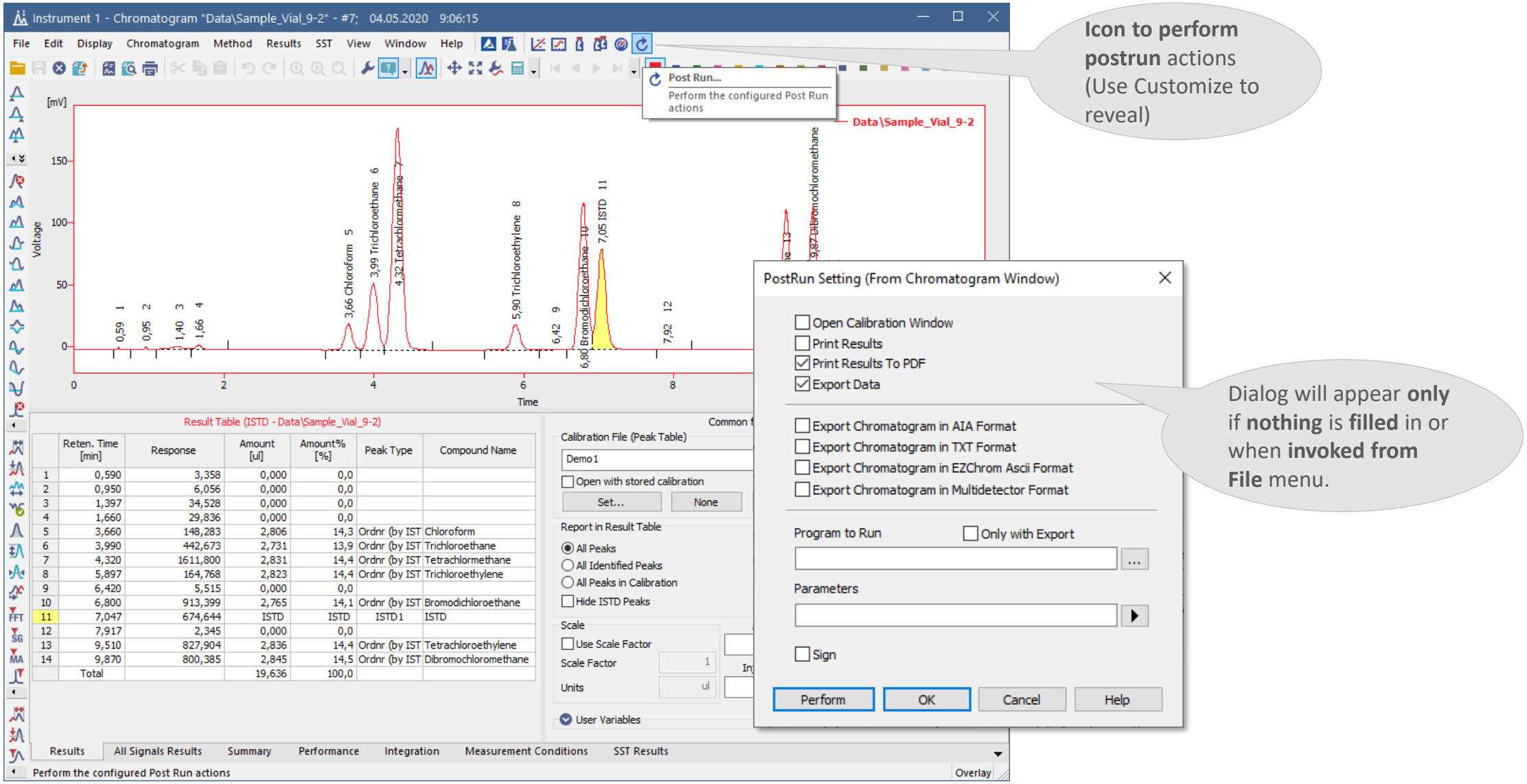
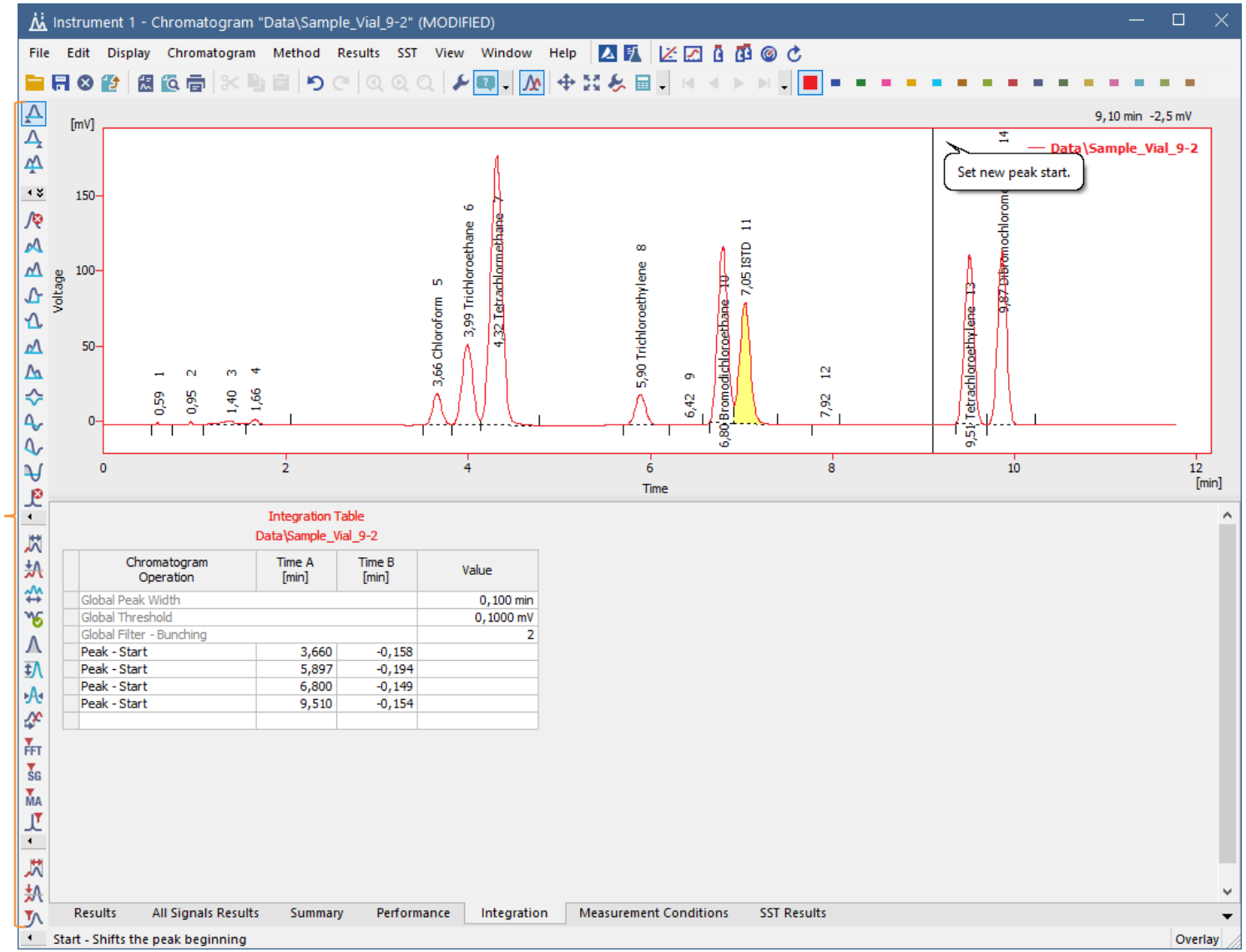

Customize
Commands
Toolbars
Menu
Options
Categories:
New Menu
File
Edit
Display
Chromatogram
Method
Results
SST
View
Window
Help
All Commands
Commands:
Global Peak Width
Global Threshold
Global Bunching
Lock
Valley
Together
Description:
Customize
Commands
Toolbars
Menu
Options
Toolbars:
Baseline
Basic
Integration
Menu Bar
Other
Overlay
Peak
Sequential Open
Standard
Reset Toolbar
New...
Rename...
Delete
Show text labels
Close
Standard
Other
Sequential Open
Overlay
Basic
Peak
Baseline
Integration
Customize...
Reset All
Customize toolbars to fit your specific needs and use
Invoked by right click in toolbar
Reset All restores original settings
[mV]
Voltage
Time
[min]
Result Table (ISTD - Data\Sample_Vial_9-2)
Reten. Time
Amount
Amount%
Common for All Signals
Calibration File (Peak Table)
Calculation


Instrument 1 - Chromatogram "Data\Sample_Vial_9-2" - #7; 04.05.2020 9:06:15
File Edit Display Chromatogram Method Results SST View Window Help
Post Run...
Perform the configured Post Run actions
Icon to perform postrun actions (Use Customize to reveal)
Data\Sample_Vial_9-2
Result Table (ISTD - Data\Sample_Vial_9-2)
Reten. Time [min] | Response | Amount [ul] | Amount% [%] | Peak Type | Compound Name
1 0,590 3,358 0,000 0,0
2 0,950 6,056 0,000 0,0
3 1,397 34,528 0,000 0,0
4 1,660 29,836 0,000 0,0
5 3,660 148,283 2,806 14,3 Ordnr (by IST Chloroform
6 3,990 442,673 2,731 13,9 Ordnr (by IST Trichloroethane
7 4,320 1611,800 2,831 14,4 Ordnr (by IST Tetrachlormethane
8 5,897 164,768 2,823 14,4 Ordnr (by IST Trichloroethylene
9 6,420 5,515 0,000 0,0
10 6,800 913,399 2,765 14,1 Ordnr (by IST Bromodichloroethane
11 7,047 674,644 ISTD ISTD ISTD1 ISTD
12 7,917 2,345 0,000 0,0
13 9,510 827,904 2,836 14,4 Ordnr (by IST Tetrachloroethylene
14 9,870 800,385 2,845 14,5 Ordnr (by IST Dibromochloromethane
Total 19,636 100,0
Calibration File (Peak Table)
Demo1
Open with stored calibration
Set... None
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Hide ISTD Peaks
Scale
Use Scale Factor
Scale Factor 1
Units ul
User Variables
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
Perform the configured Post Run actions
Overlay
PostRun Setting (From Chromatogram Window)
Open Calibration Window
Print Results
Print Results To PDF
Export Data
Export Chromatogram in AIA Format
Export Chromatogram in TXT Format
Export Chromatogram in EZChrom Ascii Format
Export Chromatogram in Multidetector Format
Program to Run
Only with Export
Parameters
Sign
Perform OK Cancel Help
Dialog will appear only if nothing is filled in or when invoked from File menu.

Ctrl while invoking command will lock it for **repeated use**. Very handy when **changing** start/end for **multiple** peaks for example.



Popular Clarity shortcuts

Graphs		General & File	
Unzoom:	**Ctrl** + [*]	Open File:	**Ctrl** + **O**
Zoom In/Out:	[+] / [−] or **Ctrl** + MOUSE WHEEL	Save File:	**Ctrl** + **S**
Zoom Vertical:	**Ctrl** + **Shift** + MOUSE WHEEL	Close File:	**Ctrl** + **W**
Move (all directions):	**Ctrl** + LEFT MOUSE BUTTON	Swap windows:	**Alt** + **Tab**
Move Left & Right:	**Shift** + MOUSE WHEEL	Copy:	**Ctrl** + **C**
Move Up & Down:	MOUSE WHEEL	Paste:	**Ctrl** + **V**

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SMART SOLUTION FOR LABORATORIES

…THANK YOU FOR YOUR TIME

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