



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**

Report Setup Chromatogram

Page Setup

- Lab. Header
- Report Header
- Method
- Calibration
- Chromatogram
- Results
- Sequence
- SST
- Audit Signatures
- Lab. Footer

Print Number of Lines: 3 Line 1: [List Icon] [List Icon] [List Icon] A

On First Page Only

Border

Gray Background

Image on the Left: Options...

Image on the Right: Options...

Clarity - Chromatography SW
DataApex
www.dataapex.com

File Name: DA.gif Browse...

Image Size:
 Original (286 x 226)
 Header Height
 Fixed Height: 15 mm Width: mm

Image Preview

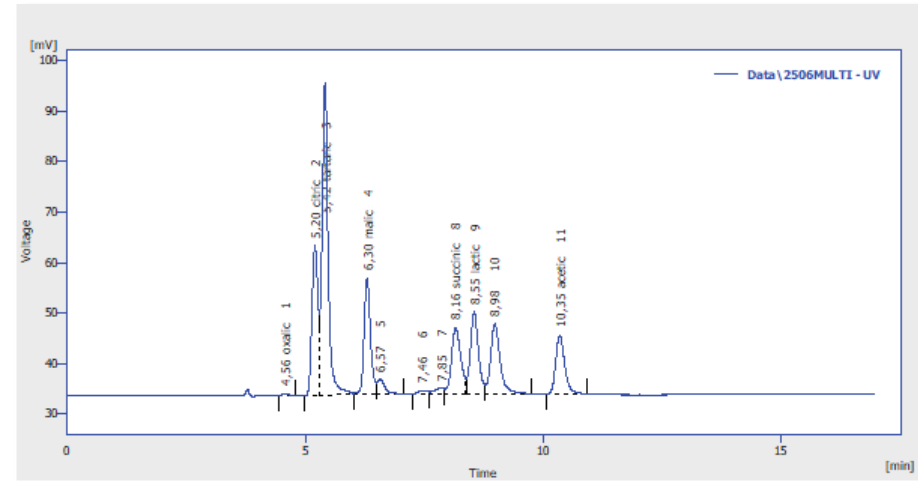
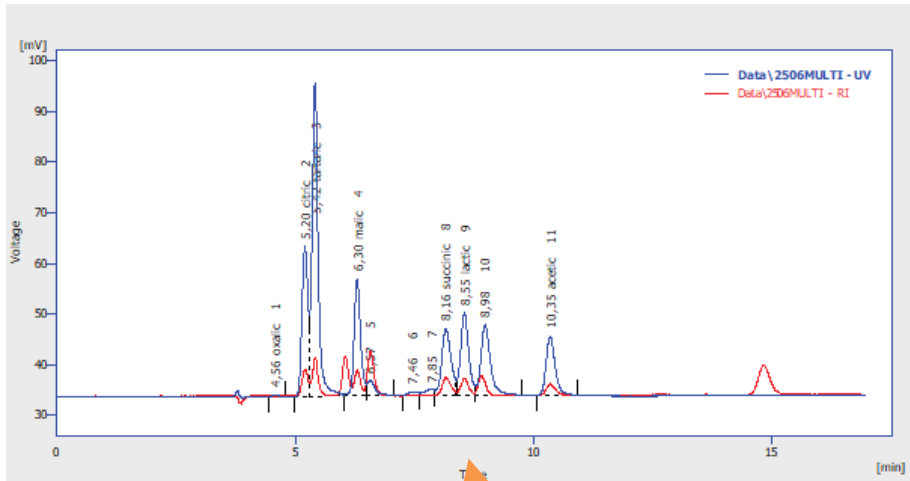
OK Cancel Help

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

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



REPORTS → TILED SIGNALS



Report Setup Chromatogram

Page Setup

- Lab. Header
- Report Header
- Method
- Calibration
- Chromatogram
- Results
- Sequence
- SST
- Audit & Signatures
- Lab. Footer

Print

- Print
- On New Page

Signals

- All
- Active Chromatogram
- Only Active Signal

Orientation

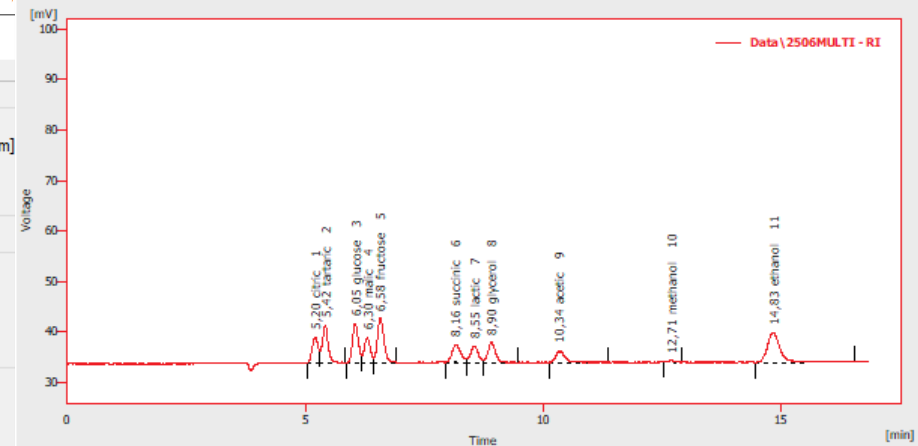
- Portrait
- Landscape
- Fixed Height: 100 [mm]
- No. of Pages: 1

Tiled by

- Signals
- Chromatograms
- not Tiled

Print Range

- As on Screen
- Whole Chromatogram
- Both



- Printer...
- Preview...
- Print...
- Print To PDF...
- Send PDF



REPORTS → ORDER OF SECTIONS

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

- Results
- All S
- Spec
- Perf
- Chro
- Sum
- V
- Table
- A
- F
- Print Op
- Print

Right click on the tab and adjust its position

11.05.2020 14:17 Chromatogram C:\Clarity\3\DataFiles\DEMO1\Data\2506MULTI.prm Page 1 of 1

Clarity - Chromatography SW
DataApex
www.dabaapex.com

Chromatogram Info:
File Name : C:\Clarity\3\DataFiles\DEMO1\Data\2506MULTI.prm
Origin : Save File C:\Clarity_2.6\DEMO1\DATA\2506MULTI.prm As C:\Clarity_2.6\DEMO1\DATA\2506MULTI.prm

Printed Version Info:
Printed Version : - #6; 04.02.2020 16:28:35, IA: 8.0 Rev.1 Recent (Linked Calibration)
Report Style : C:\Clarity\3\DataFiles\Common\Chromatogram.sly
Calibration File : C:\Clarity\3\DataFiles\DEMO1\Calib\2506HR1.cal
Project : DEMO1

Sample Description:
Sample ID : SN4616 wine
Sample : 5 ul standard wine mix 1

Method : N/A By : Administrator
Description :
Created : 01.08.2003 16:52:07 Modified : 24.04.2020 18:25:04

Result Table (ESTD - Data\2506MULTI - UV)

Reten. Time (min)	Response	Amount (µg)	Amount% (%)	Peak Type	Compound Name	
1	4,563	3,613	0,027	0,3	Ordnr	oxalic
2	5,203	253,325	1,609	16,8	Ordnr	citric
3	5,417	561,767	2,372	24,7	Ordnr	tartaric
4	6,300	217,399	1,181	12,3	Ordnr	malic
8	8,160	177,151	1,126	11,7	Ordnr	succinic
9	8,550	193,934	1,970	20,5	Ordnr	lactic
11	10,347	152,602	1,312	13,7	Ordnr	acetic
C11	12,710					methanolic
Total			9,596	100,0		

11.05.2020 14:18 Chromatogram C:\Clarity\3\DataFiles\DEMO1\Data\2506MULTI.prm Page 1 of 1

Clarity - Chromatography SW
DataApex
www.dabaapex.com

Result Table (ESTD - Data\2506MULTI - UV)

Reten. Time (min)	Response	Amount (µg)	Amount% (%)	Peak Type	Compound Name	
1	4,563	3,613	0,027	0,3	Ordnr	oxalic
2	5,203	253,325	1,609	16,8	Ordnr	citric
3	5,417	561,767	2,372	24,7	Ordnr	tartaric
4	6,300	217,399	1,181	12,3	Ordnr	malic
8	8,160	177,151	1,126	11,7	Ordnr	succinic
9	8,550	193,934	1,970	20,5	Ordnr	lactic
11	10,347	152,602	1,312	13,7	Ordnr	acetic
C11	12,710					methanolic
Total			9,596	100,0		

Chromatogram Info:
File Name : C:\Clarity\3\DataFiles\DEMO1\Data\2506MULTI.prm
Origin : Save File C:\Clarity_2.6\DEMO1\DATA\2506MULTI.prm As C:\Clarity_2.6\DEMO1\DATA\2506MULTI.prm
File Created : 24.04.2020 18:25:04
Acquired Date : 01.08.2003 16:52:07
By : DataApex

Printed Version Info:
Printed Version : - #6; 04.02.2020 16:28:35, IA: 8.0 Rev.1 Recent (Linked Calibration)
Report Style : C:\Clarity\3\DataFiles\Common\Chromatogram.sly
Calibration File : C:\Clarity\3\DataFiles\DEMO1\Calib\2506HR1.cal
Project : DEMO1
Printed Date : 11.05.2020 14:18:28
By : Admin

Sample Description:
Sample ID : SN4616 wine
Sample : 5 ul standard wine mix 1

Method : N/A By : Administrator
Description :
Created : 01.08.2003 16:52:07 Modified : 24.04.2020 18:25:04



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

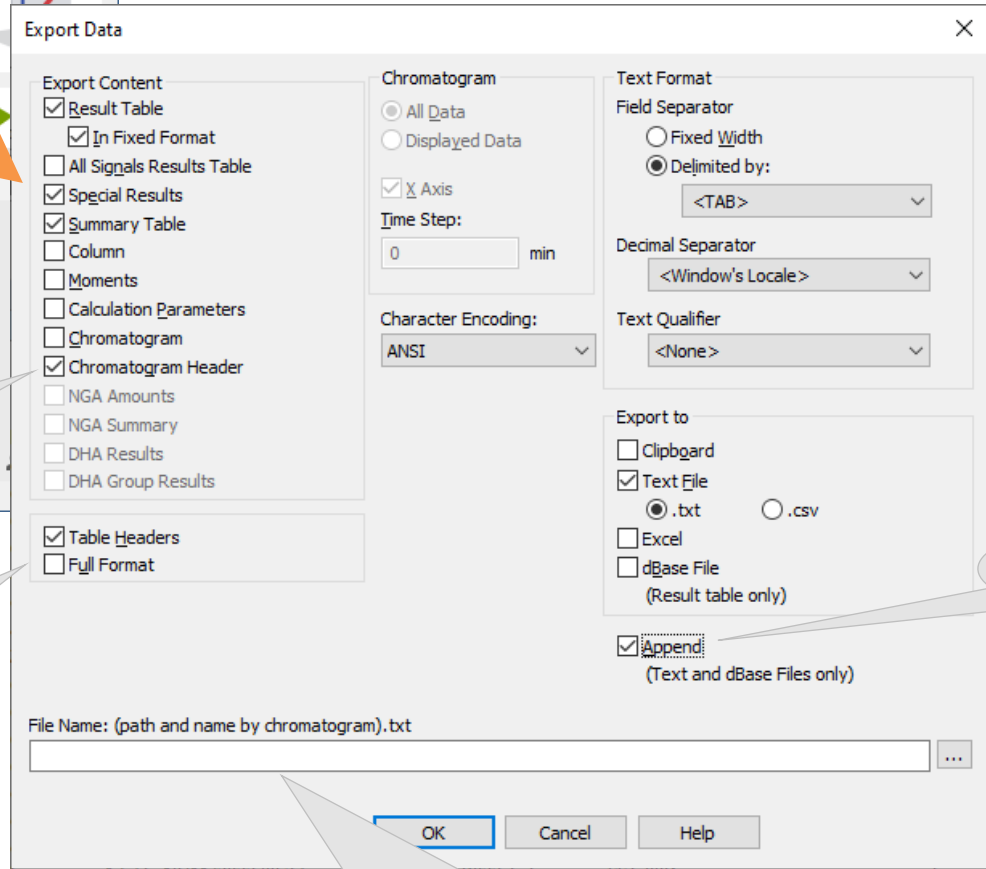
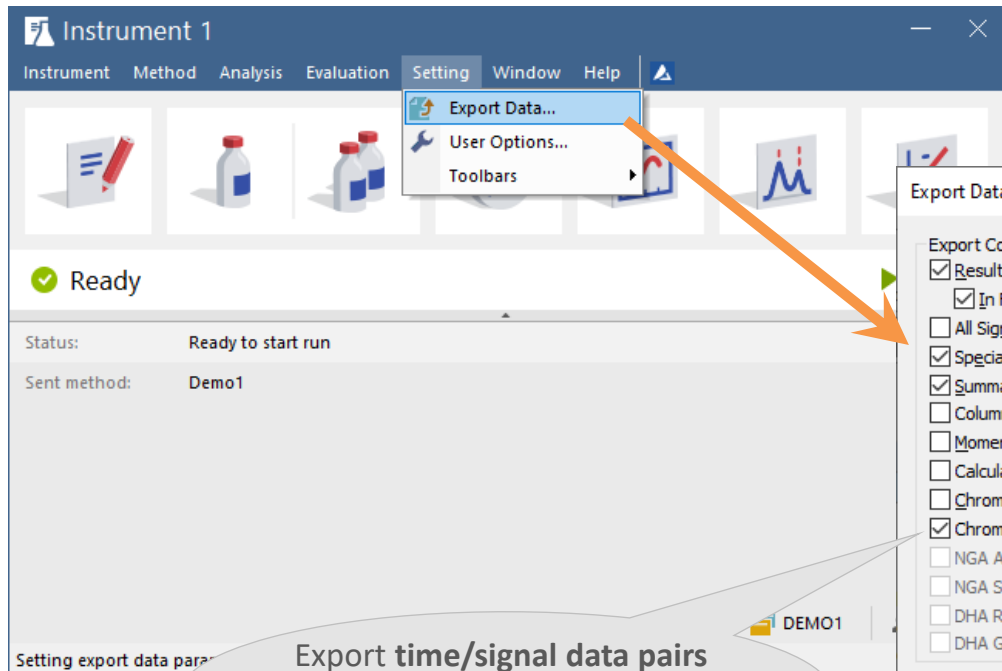


Export data

- **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

The screenshot shows a chromatogram window with a plot of detector response versus time (min). The plot displays several peaks labeled with their retention times and compound names: 4 (Chloroform), 5 (Trichloroethane), 6 (Tetrachloroethane), 7 (Trichloroethylene), 8, 9 (Bromodichloroethane), 10 (ISTD), 11, 12 (Tetrachloroethylene), and 13 (Dibromochloromethane). The x-axis ranges from 0 to 12 minutes. The y-axis represents detector response.

The 'Export' menu is open, showing options: Export Data..., Export Chromatogram..., Export Summary Table..., Export as Picture to Clipboard, and Export as Picture to File... The 'Export as Picture to Clipboard' option is highlighted.

The results table below the plot shows the following data:

Peak	Amount	Amount% [%]	Peak Type	Compound Name		
1	0,000	0,0				
2	0,000	0,0				
3	0,000	0,0				
4	2,842	14,2	Ordnr (by ISTD)	Chloroform		
5	2,770	13,9	Ordnr (by ISTD)	Trichloroethane		
6	2,899	14,5	Ordnr (by ISTD)	Tetrachloromethane		
7	2,863	14,3	Ordnr (by ISTD)	Trichloroethylene		
8	0,000	0,0				
9	2,823	14,1	Ordnr (by ISTD)	Bromodichloroethane		
10	ISTD	ISTD	ISTD1	ISTD		
11	0,000	0,0				
12	9,500	78,185	2,895	14,5	Ordnr (by ISTD)	Tetrachloroethylene
13	9,860	763,085	2,905	14,5	Ordnr (by ISTD)	Dibromochloromethane
Total		19,997	100,0			

The 'Common for All Signals' settings panel is visible, showing 'Calculation' set to 'ISTD' and 'Integration Algorithm' set to '8.0'. The 'Report in Result Table' section has 'All Peaks' selected. The 'Unidentified peaks' section has 'Response Base' set to 'Area' and 'Response Factor' set to '0'. The 'Scale' section has 'Scale Factor' set to '1' and 'Units' set to 'ul'. The 'Inj. Volume [uL]' is set to '1000' and 'Dilution' is set to '1'.

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)

Automatic export of data using the post run function

Export according to Settings - Export Data

Possibility to export chromatogram to different formats

Single Analysis

- Open Chromatogram Window
- Open Calibration Window
- Print Results
- Print Results To PDF
- Export Data
- Open Chromatogram with stored Calibration
- Include Chromatogram in SST

Report Style: Analysis

- 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: [] ▶

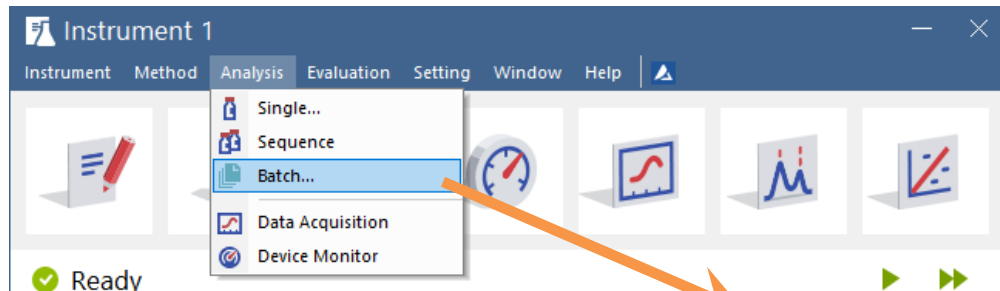
Analysis | **Post Run Settings** | User Variables

Control: [Send method] [Run] [Stop] [Abort] [Snapshot]

Chromatogram File Name (Data\Instrument 1 - 20.04.2022 15_36_03): %e - %R

Enable File Overwrite Counter: 1 Data Recovery...

OK Cancel Help



Automatically export data from multiple chromatograms using the Batch dialog

Export according to Settings - Export Data

Batch dialog box showing a list of files and options for export.

Status: Ready to start run
Sent method: Demo1

View batch dialog

File Type: Chromatograms

Select All / Unselect All

Sort by: Name (selected), Time

Order: Normal (selected), Backward

Options:

- Reprocess by Method
- Complete Processing
- Open Chromatogram Window
- Preserve Integration
- Open Calibration Window
- Print Results
- 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

Parameters: []

Proceed / Cancel / Help

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**

Export according to **Settings - Export Data**



EXPORT DATA → TEXT FILE FORMAT

1	2	3	4	5	6	7	8	9	10		
Signal No.	Signal Name	Peak No.	Reten. time	Response	Response Base	Amount [ul]	Amount [%]	Peak Type	Compound Name		
1		1	0,573	8,983	A	0	0				
2		2	1,383	32,419	A	0	0				
3		3	1,647	26,928	A	0	0				
4		4	3,647	140,237	A	2,8417	14,211	Ordnr (by ISTD1)	Chloroform		
5		5	3,983	419,318	A	2,7704	13,854	Ordnr (by ISTD1)	Trichloroethane		
6		6	4,307	1541,388	A	2,8993	14,499	Ordnr (by ISTD1)	Tetrachlormethane		
7		7	5,883	156,032	A	2,8626	14,315	Ordnr (by ISTD1)	Trichloroethylene		
8		8	6,403	5,169	A	0	0				
9		9	6,79	870,847	A	2,8234	14,119	Ordnr (by ISTD1)	Bromodichloroethane		
10		10	7,033	629,957	A						
11		11	7,903	2,25	A						
12		12	9,5	789,185	A						
13		13	9,86	763,085	A						
14			Total								
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

Export Content

- Result Table
 - In Fixed Format
 - All Signals Results Table
- Special Results
- Summary Table
- Column
- Moments
- Calculation Parameters
- Chromatogram
- Chromatogram Header
 - NGA Amounts
 - NGA Summary
 - DHA Results
 - DHA Group Results
- Table Headers
- Full Format

Chromatogram

- All Data
- Displayed Data
- X Axis
- Time Step: min
- Character Encoding: ANSI

Text Format

Field Separator

- Fixed Width
- Delimited by: <TAB>

Decimal Separator: <Window's Locale>

Text Qualifier: <None>

Export to

- Clipboard
- Text File
 - .txt
 - .csv
- Excel
- dBase File (Result table only)

Append (Text and dBase Files only)

File Name: (path and name by chromatogram).txt

OK Cancel Help

PPT EXPORT DATA → EXCEL (*.XLSX) FORMAT

Export Data

Export Content

- Result Table
- In Fixed Format
- All Signals Results Table
- Special Results
- Summary Table
- Column
- Moments
- Calculation Parameters
- Chromatogram
- Chromatogram Header
- NGA Amounts
- NGA Summary
- DHA Results
- DHA Group Results

Chromatogram

- All Data
- Displayed Data
- X Axis
- Time Step: 0 min

Character Encoding: ANSI

Text Format

Field Separator: Fixed Width, Delimited by: <TAB>

Decimal Separator: <Window's Locale>

Text Qualifier: <None>

Export to

- Clipboard
- Text File
- Excel
- dBase File (Result table only)

Append (Text and dBase Files only)

File Name: (path and name by chromatogram).xlsx

OK Cancel Help

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



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- Perform postrun
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- Most popular shortcuts



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_6-2
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

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

File Type: Chromatograms

Target Folder Name: C:\Archive\

Calibration Standards
 From Common
 Including Common

Without Compressing
 Move to Archive

OK Cancel Archive Help

Restore archived data

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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The screenshot displays a chromatogram with a red trace showing peaks at various retention times. The x-axis is labeled 'Time [min]' and ranges from 0 to 12. The y-axis is labeled 'Voltage [mV]' and ranges from 0 to 150. Several peaks are identified with their retention times and names: 0.59, 0.95, 1.40, 1.66, 3.66 Chloro, 3.99, 4.32, 5.90 Trichloro, 6.42, 6.80 Bromodichloroetha, 7.92, 9.51 Tetrachloroethylene. A 'Customize' dialog box is open, showing the 'Toolbars' tab. The 'Toolbars' list includes: Baseline, Basic, Integration, Menu Bar, Other, Overlay, Peak, Sequential Open, and Standard. A 'Reset All' button is visible at the bottom of the dialog. A context menu is also open over the toolbar, listing the same categories and including a 'Customize...' button. A 'Result Table (ISTD - Data\Sample_Vial_9-2)' is visible at the bottom of the interface.

Customize toolbars to fit your specific needs and use

Invoked by right click in toolbar

Reset All restores original settings



ADVANCED TRAINING → TIPS & TRICKS → PERFORM POSTRUN

The screenshot shows the 'Instrument 1 - Chromatogram' window. The main plot displays Voltage [mV] vs Time [min] with several peaks labeled. Below the plot is a 'Result Table (ISTD - Data\Sample_Vial_9-2)'. A 'Post Run...' tooltip is visible over a toolbar icon. A 'PostRun Setting (From Chromatogram Window)' dialog box is open, showing various options for post-run actions.

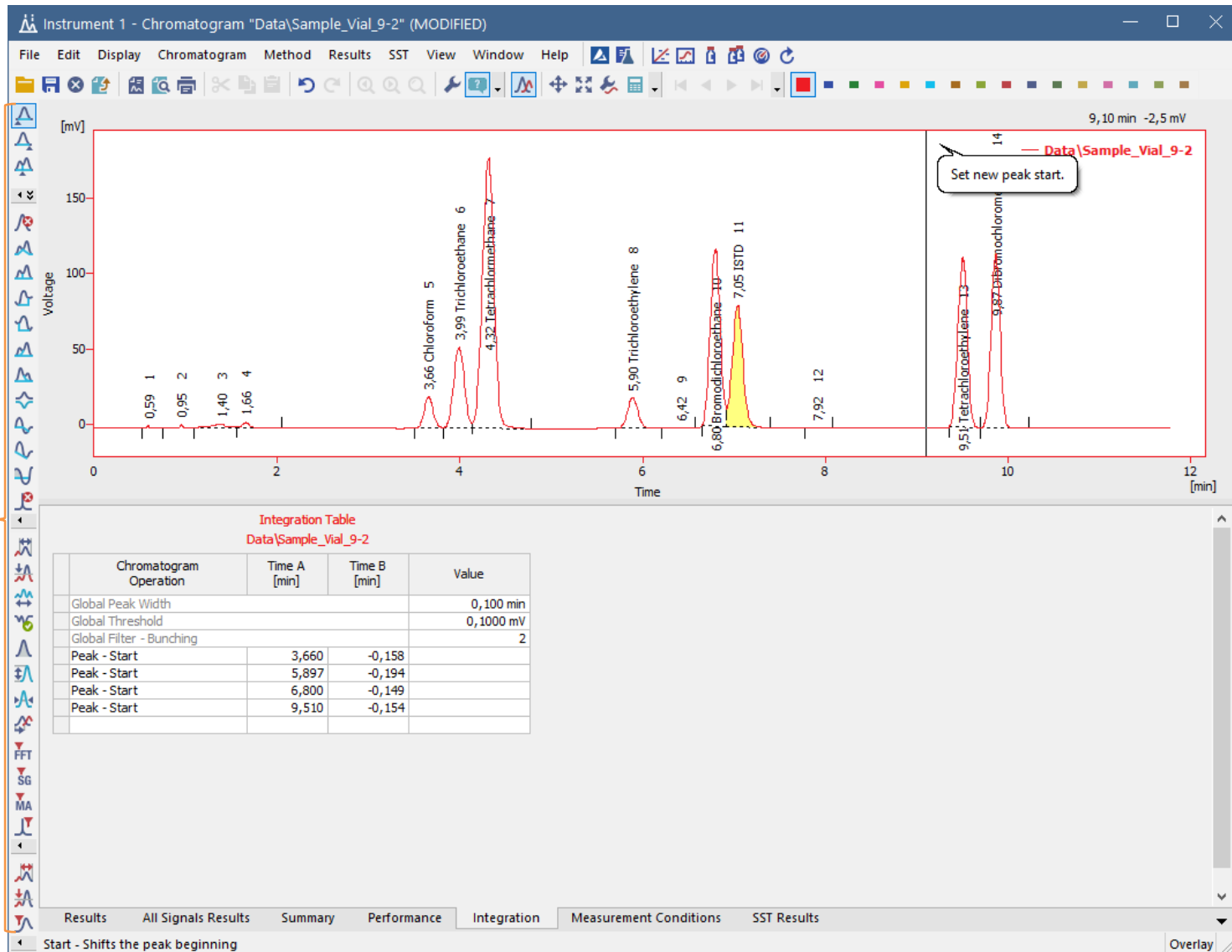
Reten. Time [min]	Response	Amount [ul]	Amount% [%]	Peak Type	Compound Name
1	0,590	3,358	0,000	0,0	
2	0,950	6,056	0,000	0,0	
3	1,397	34,528	0,000	0,0	
4	1,660	29,836	0,000	0,0	
5	3,660	148,283	2,806	14,3	Ordnr (by IST Chloroform
6	3,990	442,673	2,731	13,9	Ordnr (by IST Trichloroethane
7	4,320	1611,800	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	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		

Icon to perform postrun actions (Use Customize to reveal)

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

Unzoom:	Ctrl +
Zoom In/Out:	/ or Ctrl + MOUSE WHEEL
Zoom Vertical:	Ctrl + Shift + MOUSE WHEEL
Move (all directions):	Ctrl + LEFT MOUSE BUTTON
Move Left & Right:	Shift + MOUSE WHEEL
Move Up & Down:	MOUSE WHEEL

General & File

Open File:	Ctrl + O
Save File:	Ctrl + S
Close File:	Ctrl + W
Swap windows:	Alt + Tab
Copy:	Ctrl + C
Paste:	Ctrl + V



...THANK YOU FOR YOUR TIME



SUPPORT@DATAAPEX.COM
WWW.DATAAPEX.COM