23.0331

Clarity™

ADVANCED CHROMATOGRAPHY SOFTWARE

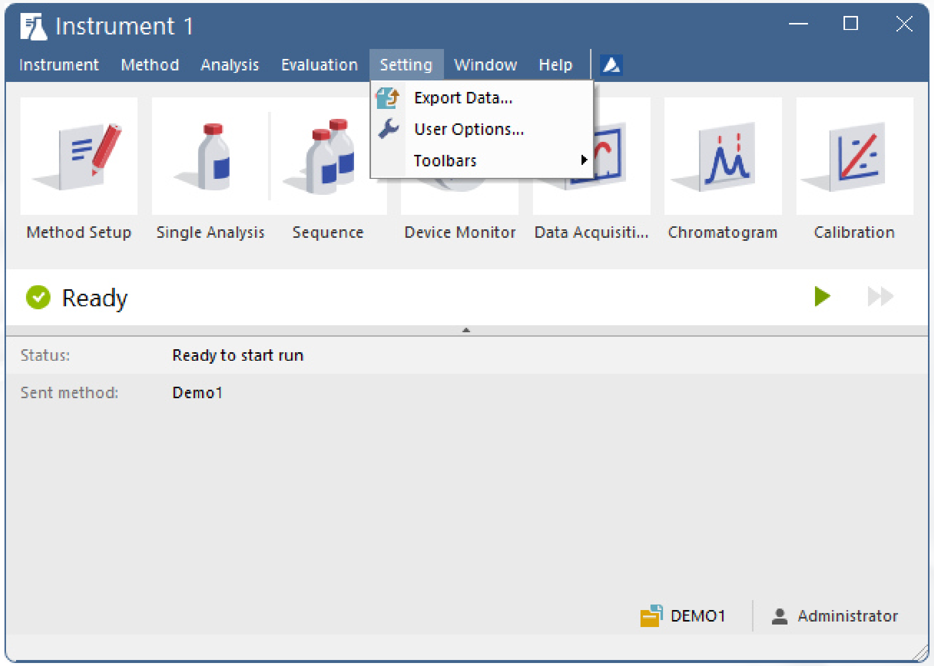
CLARITY TRAINING

ADVANCED – PART 1

DataApex

AGENDA

- Instrument window
    - User Options
- Single Analysis
    - Injected volume
    - Autosampler use
- Sequence table
    - Sequence Mode
    - Options
    - Import, Fill series

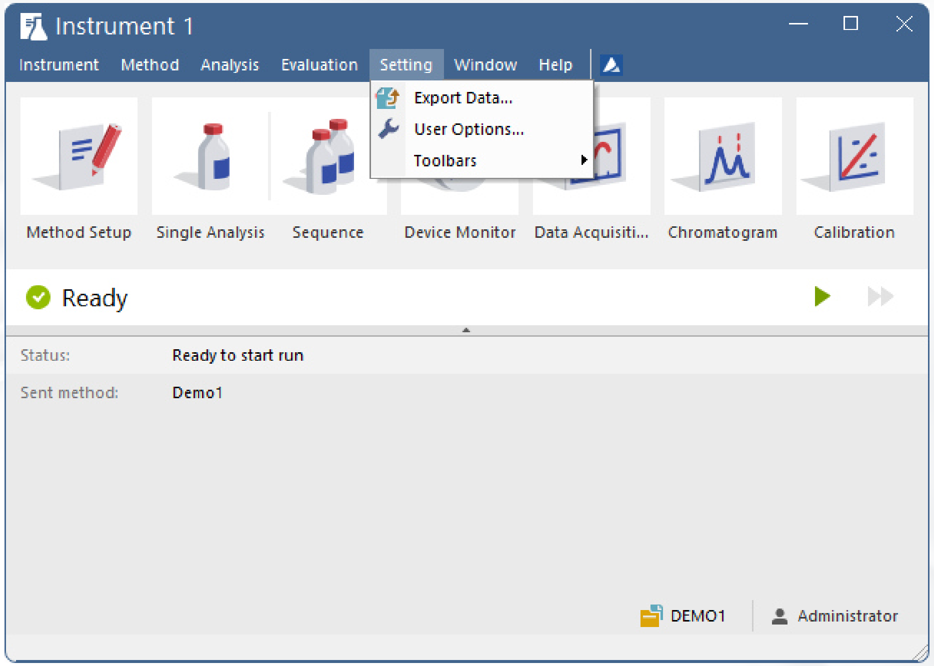


Status: Ready to start run

Sent method: Demo1

AGENDA

- Instrument window
    - User Options
- Single Analysis
    - Injected volume
    - Autosampler use
- Sequence table
    - Sequence Mode
    - Options
    - Import, Fill series



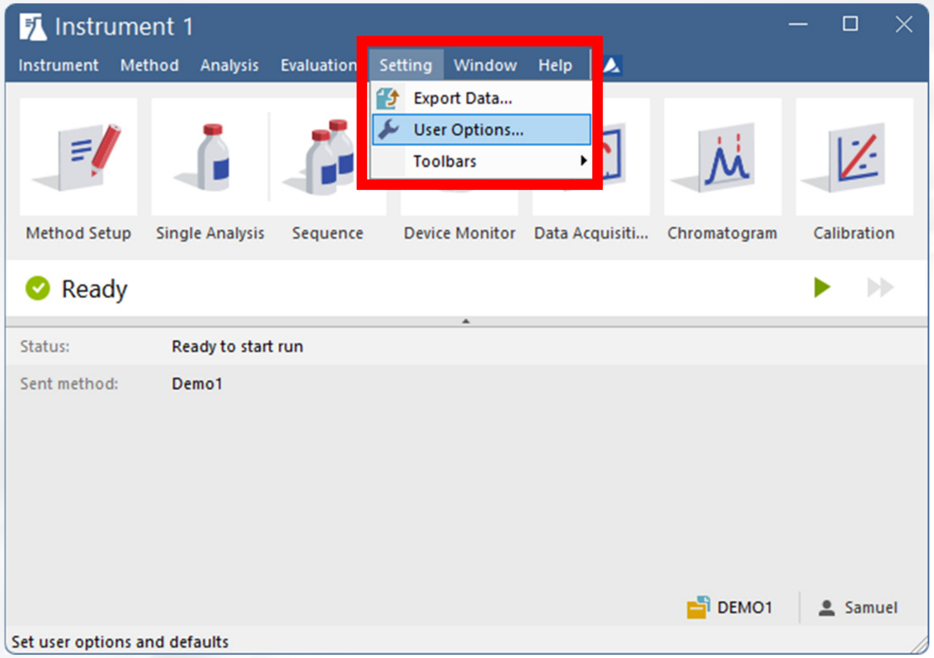
Status: Ready to start run

Sent method: Demo1

INSTRUMENT WINDOW

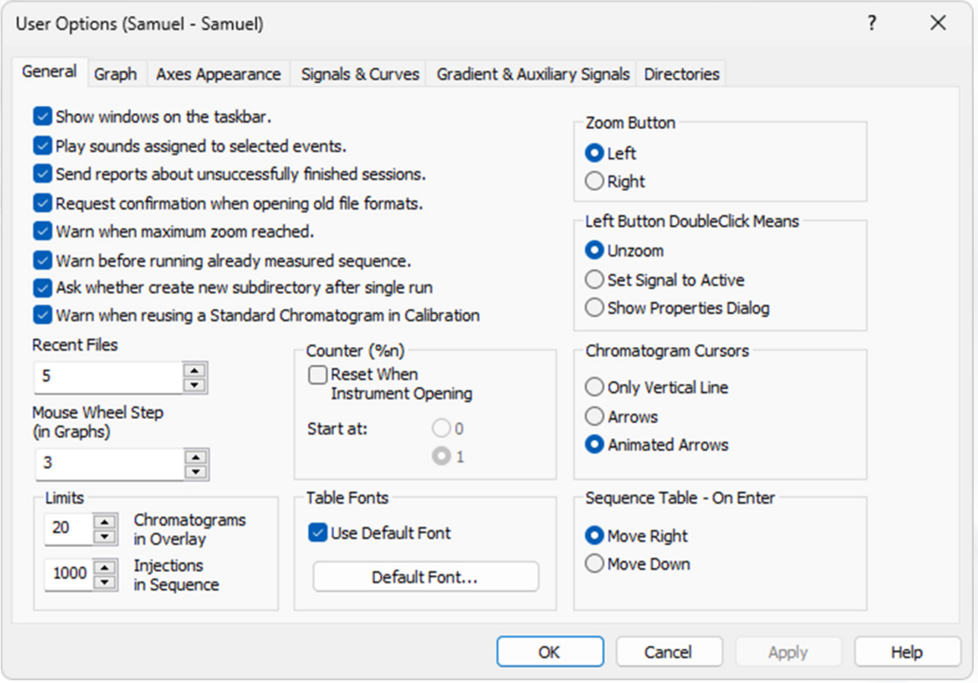
USER OPTIONS

- Stored in desktop *.dsk files = can be set individually for each user
- Shared desktop file to share settings



Status: Ready to start run

Sent method: Demo1



☑ Show windows on the taskbar.
☑ Play sounds assigned to selected events.
☑ Send reports about unsuccessfully finished sessions.
☑ Request confirmation when opening old file formats.
☑ Warn when maximum zoom reached.
☑ Warn before running already measured sequence.
☑ Ask whether create new subdirectory after single run
☑ Warn when reusing a Standard Chromatogram in Calibration

Recent Files: 5

Mouse Wheel Step (in Graphs): 3

Limits
20 Chromatograms in Overlay
1000 Injections in Sequence

Counter (%n)
☐ Reset When Instrument Opening
Start at: ○ 0 ● 1

Table Fonts
☑ Use Default Font
Default Font...

Zoom Button
● Left
○ Right

Left Button DoubleClick Means
● Unzoom
○ Set Signal to Active
○ Show Properties Dialog

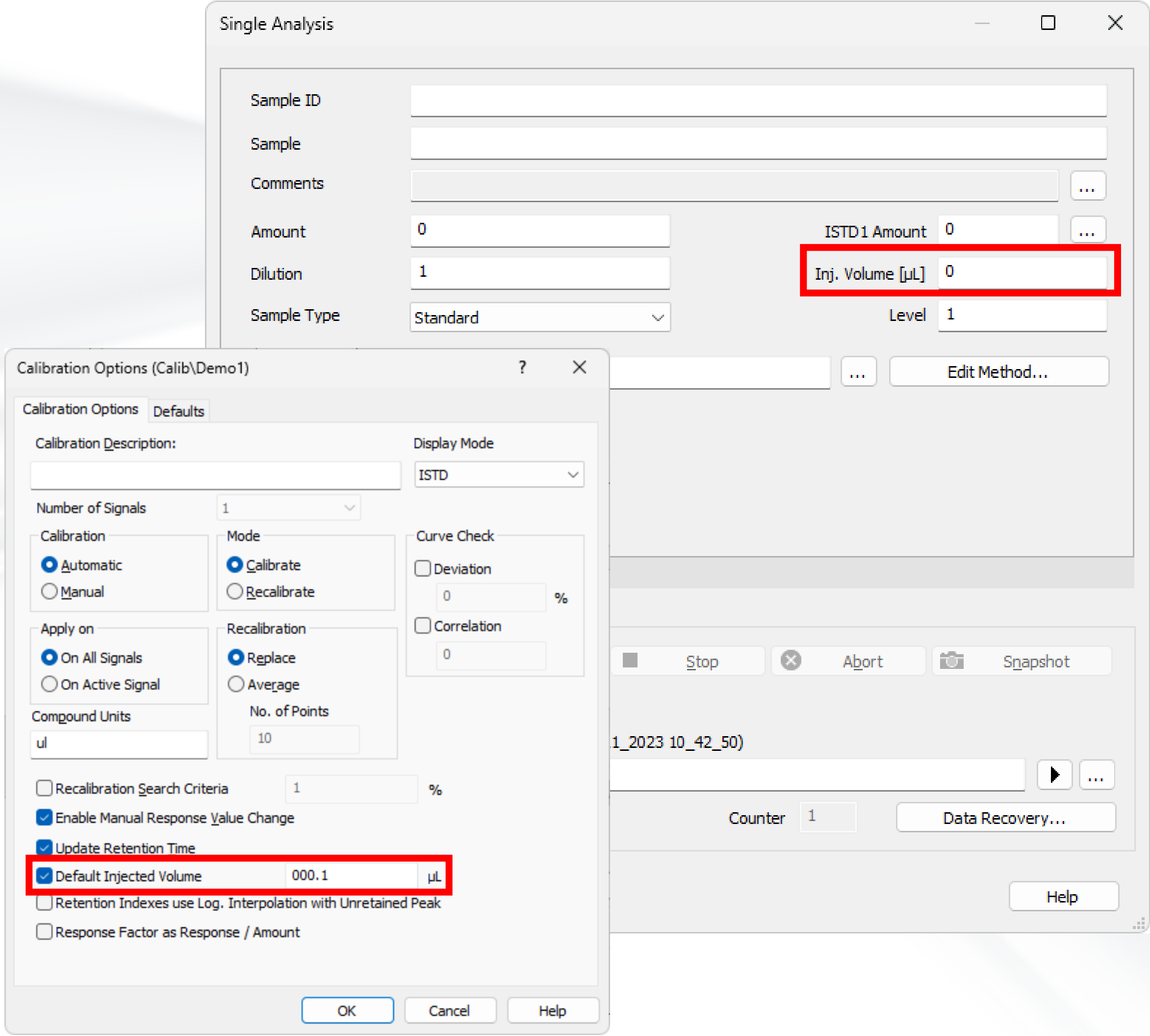
Chromatogram Cursors
○ Only Vertical Line
○ Arrows
● Animated Arrows

Sequence Table - On Enter
● Move Right
○ Move Down

SINGLE ANALYSIS

INJECTED VOLUME

- **Linear** detector response is considered
- First, set Default Injected Volume in Calibration Options
- In Single Analysis, set the Injection volume for the sample and standard
- The responses are corrected by the ratio of Inj. Volume and Default Injected Volume in recalibration or calibration calculations



Single Analysis

Sample ID
Sample
Comments
Amount 0
ISTD1 Amount 0
Dilution 1
Inj. Volume [μL] 0
Sample Type Standard
Level 1
1_2023 10_42_50)
Counter 1

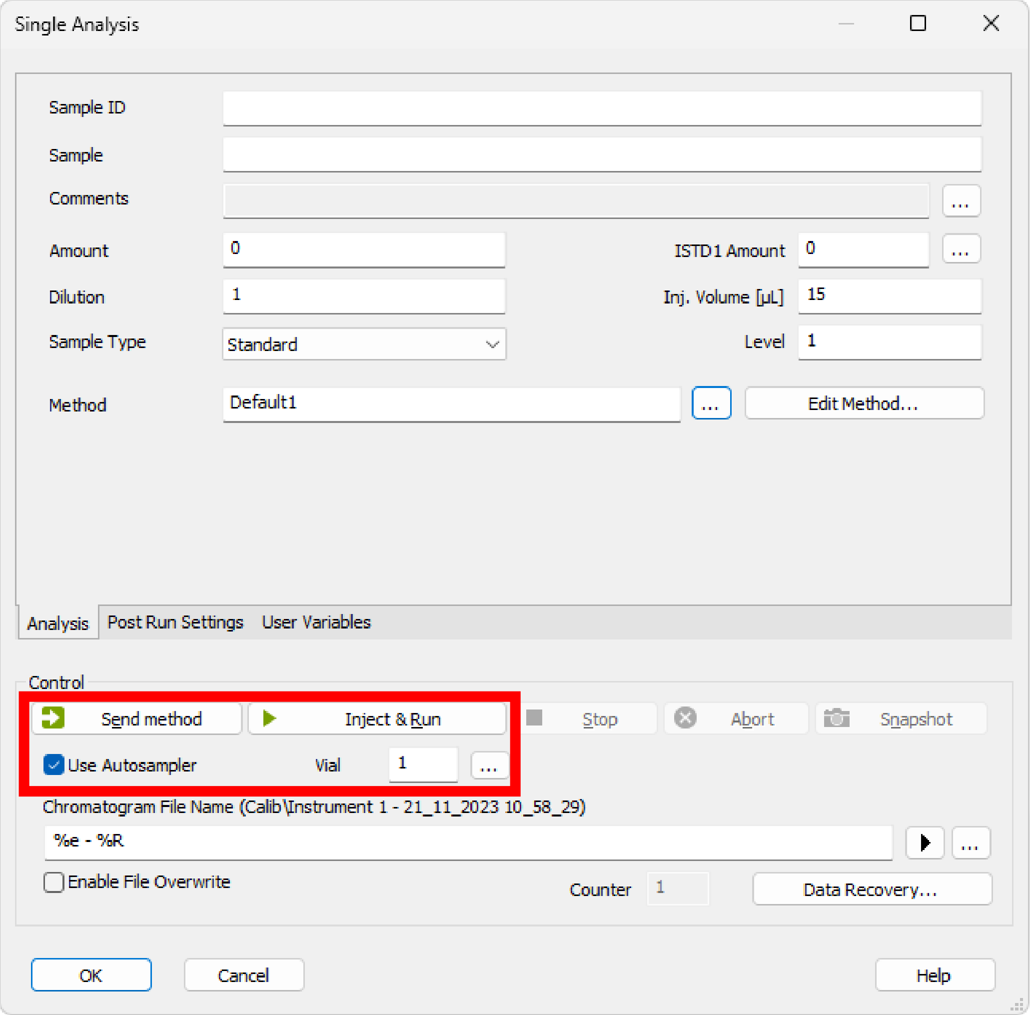
Calibration Options (Calib\Demo1)

Calibration Description:
Display Mode ISTD
Number of Signals 1
Calibration: ● Automatic ○ Manual
Mode: ● Calibrate ○ Recalibrate
Curve Check: ☐ Deviation 0 % ☐ Correlation 0
Apply on: ● On All Signals ○ On Active Signal
Recalibration: ● Replace ○ Average
No. of Points 10
Compound Units ul
☐ Recalibration Search Criteria 1 %
☑ Enable Manual Response Value Change
☑ Update Retention Time
☑ Default Injected Volume 000.1 μL
☐ Retention Indexes use Log. Interpolation with Unretained Peak
☐ Response Factor as Response / Amount

SINGLE ANALYSIS

AUTOSAMPLER USE

- **Inject & Run** performs one injection from the specified vial and starts the acquisition
- Vial can be selected via a graphic interface if supported by the AS
- The **Use Autosampler** checkbox is present only if AS is configured



Single Analysis

Sample ID:

Sample:

Comments:

Amount: 0

ISTD1 Amount: 0

Dilution: 1

Inj. Volume [µL]: 15

Sample Type: Standard

Level: 1

Method: Default1

☑ Use Autosampler

Vial: 1

Chromatogram File Name (Calib\Instrument 1 - 21_11_2023 10_58_29)

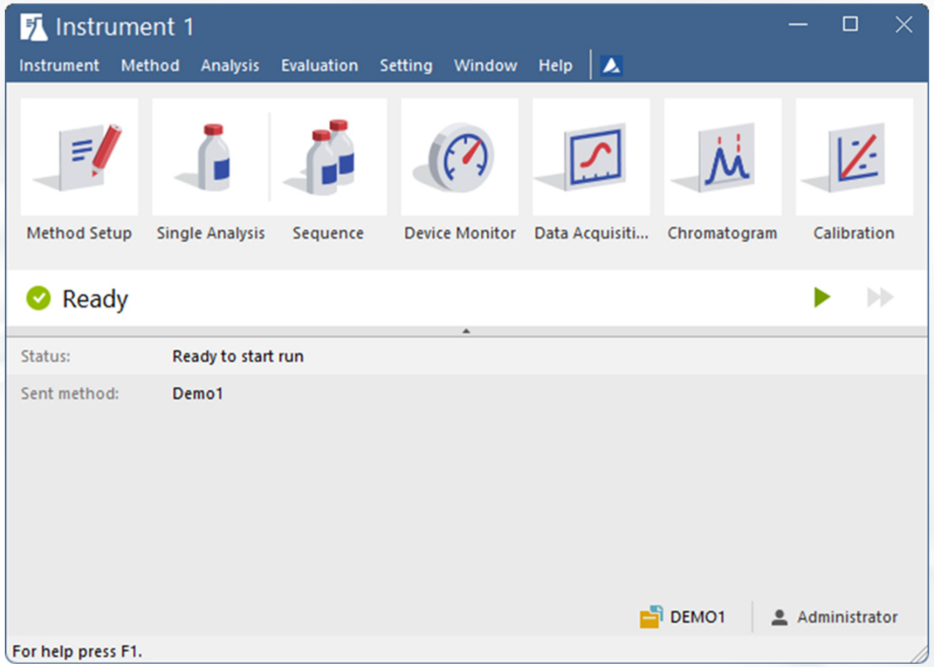
%e - %R

☐ Enable File Overwrite

Counter: 1

AGENDA

- Instrument window
  - User Options
- Single Analysis
  - Injected volume
  - Autosampler use
- Sequence
  - Description
  - Options and functions overview
  - Import, Fill series, Select vial



Status: Ready to start run

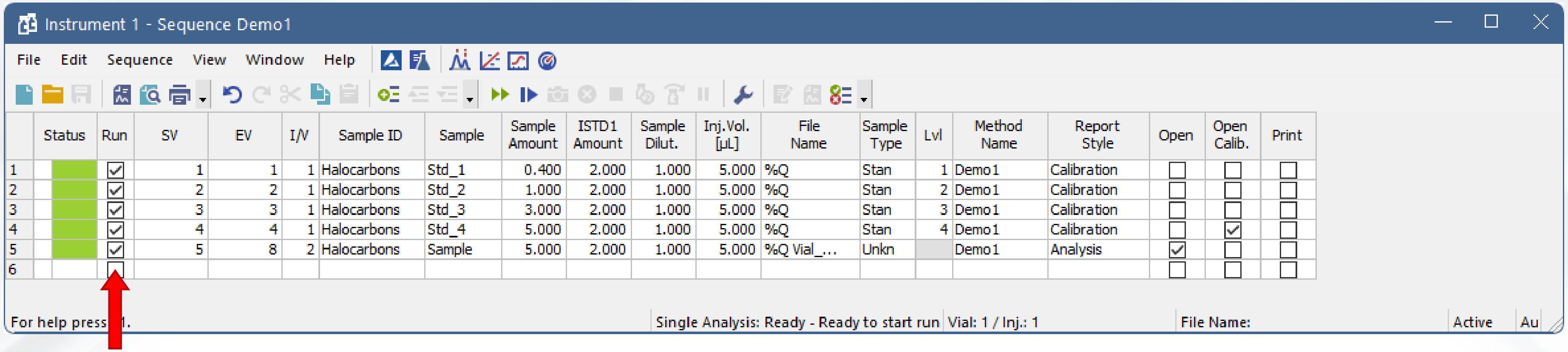
Sent method: Demo1

For help press F1.

SEQUENCE TABLE OVERVIEW

ADD SAMPLES

- Samples are added by filling the **last empty row**
  - When any field is filled, the other fields are **copied** from the previous row
- **Copy & Paste** one or more rows to add samples
- Import of sample data from **text files**
- **Reprocessing** of the 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	Halocarbons	Std_1	0.400	2.000	1.000	5.000	%Q	Stan	1	Demo1	Calibration	☐	☐	☐
2	🟩	☑	2	2	1	Halocarbons	Std_2	1.000	2.000	1.000	5.000	%Q	Stan	2	Demo1	Calibration	☐	☐	☐
3	🟩	☑	3	3	1	Halocarbons	Std_3	3.000	2.000	1.000	5.000	%Q	Stan	3	Demo1	Calibration	☐	☐	☐
4	🟩	☑	4	4	1	Halocarbons	Std_4	5.000	2.000	1.000	5.000	%Q	Stan	4	Demo1	Calibration	☐	☑	☐
5	🟩	☑	5	8	2	Halocarbons	Sample	5.000	2.000	1.000	5.000	%Q Vial_…	Unkn		Demo1	Analysis	☑	☐	☐
6		☐															☐	☐	☐

For help press 1.

Single Analysis: Ready - Ready to start run

Vial: 1 / Inj.: 1

File Name:

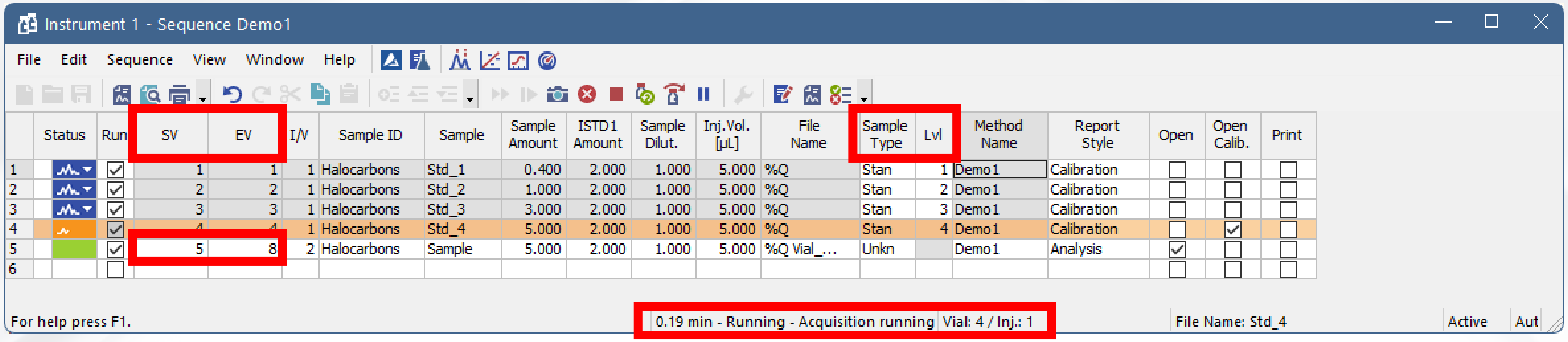
Active

Au

SEQUENCE WINDOW

DESCRIPTION

- **SV, EV** = start and end vial injection number
  - A single row can define **several** vials/injections
- **Sample Type, Lvl** = can be used for automatic **recalibration** via sequence
- Window bottom shows the **state** of the sequence (runtime, vial, etc.)



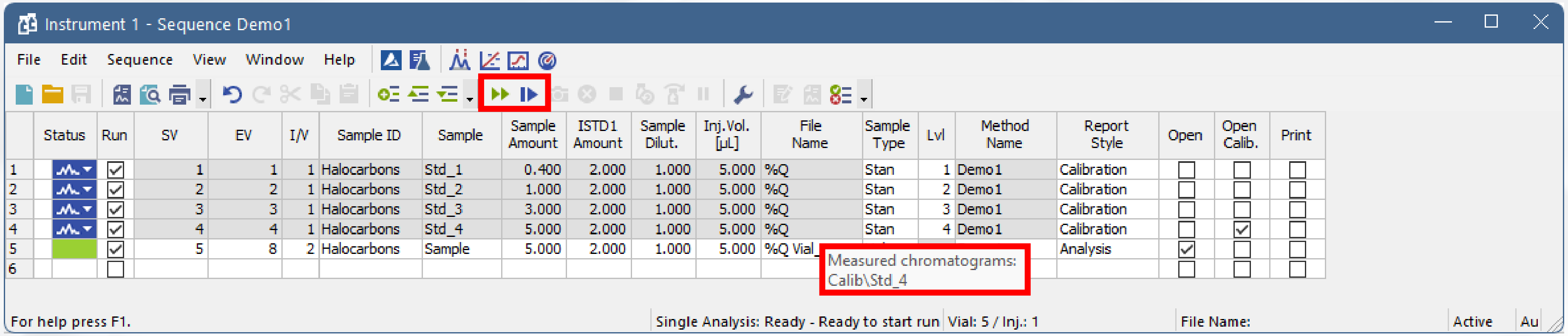
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1		☑	1	1	1	Halocarbons	Std_1	0.400	2.000	1.000	5.000	%Q	Stan	1	Demo1	Calibration	☐	☐	☐
2		☑	2	2	1	Halocarbons	Std_2	1.000	2.000	1.000	5.000	%Q	Stan	2	Demo1	Calibration	☐	☐	☐
3		☑	3	3	1	Halocarbons	Std_3	3.000	2.000	1.000	5.000	%Q	Stan	3	Demo1	Calibration	☐	☐	☐
4		☑	4	4	1	Halocarbons	Std_4	5.000	2.000	1.000	5.000	%Q	Stan	4	Demo1	Calibration	☐	☑	☐
5		☑	5	8	2	Halocarbons	Sample	5.000	2.000	1.000	5.000	%Q Vial_...	Unkn		Demo1	Analysis	☑	☐	☐
6		☐															☐	☐	☐

For help press F1. | 0.19 min - Running - Acquisition running | Vial: 4 / Inj.: 1 | File Name: Std_4 | Active | Aut

SEQUENCE WINDOW

DESCRIPTION

- **Run** sequence using Ctrl+Q or the ⏩ icon
    - Running sequence will lead to a reset of all rows (indicated by a message dialog)
- **Resume** sequence Ctrl+Space or the ⏯ icon
    - Continue from the first unmeasured row with the Run option checked
- Tooltips display additional details (e.g., actual file names of measured chromatograms, etc.)



	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	Halocarbons	Std_1	0.400	2.000	1.000	5.000	%Q	Stan	1	Demo1	Calibration	☐	☐	☐
2		☑	2	2	1	Halocarbons	Std_2	1.000	2.000	1.000	5.000	%Q	Stan	2	Demo1	Calibration	☐	☐	☐
3		☑	3	3	1	Halocarbons	Std_3	3.000	2.000	1.000	5.000	%Q	Stan	3	Demo1	Calibration	☐	☐	☐
4		☑	4	4	1	Halocarbons	Std_4	5.000	2.000	1.000	5.000	%Q	Stan	4	Demo1	Calibration	☐	☑	☐
5	🟩	☑	5	8	2	Halocarbons	Sample	5.000	2.000	1.000	5.000	%Q Vial_				Analysis	☑	☐	☐
6		☐															☐	☐	☐

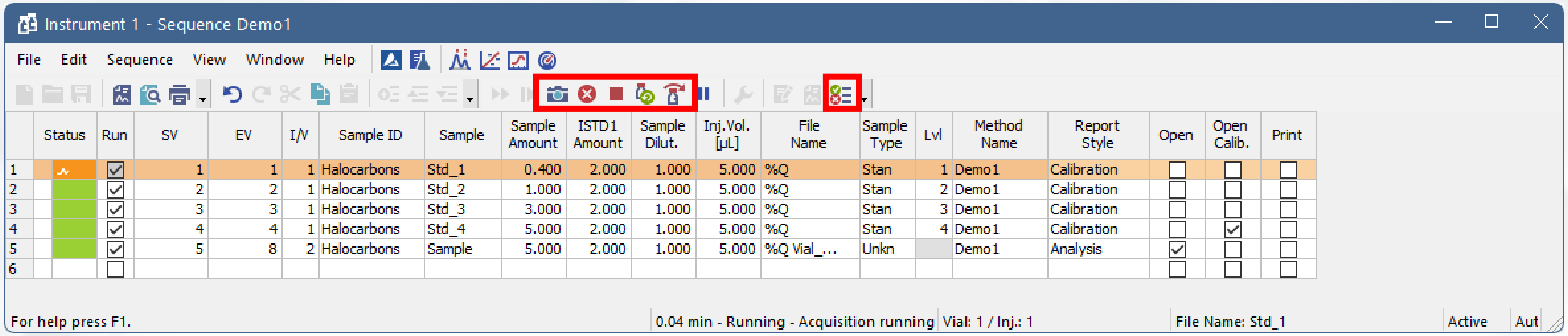
Measured chromatograms:
Calib\Std_4

For help press F1. | Single Analysis: Ready - Ready to start run | Vial: 5 / Inj.: 1 | File Name: | Active | Au

SEQUENCE WINDOW

BASIC FUNCTIONS

- **Snapshot** 📷: create a temporary snapshot (will be replaced by the complete chromatogram when measured)
- **Abort** sequence ⊗: terminate the sequence without saving the current chromatogram
- **Stop** sequence ■: 1st click halts the sequence after the current measurement, 2nd click stops analysis immediately
- **Repeat injection**: interrupt the actual measurement and repeat injection
- **Skip vial**
- **Check sequence** for errors



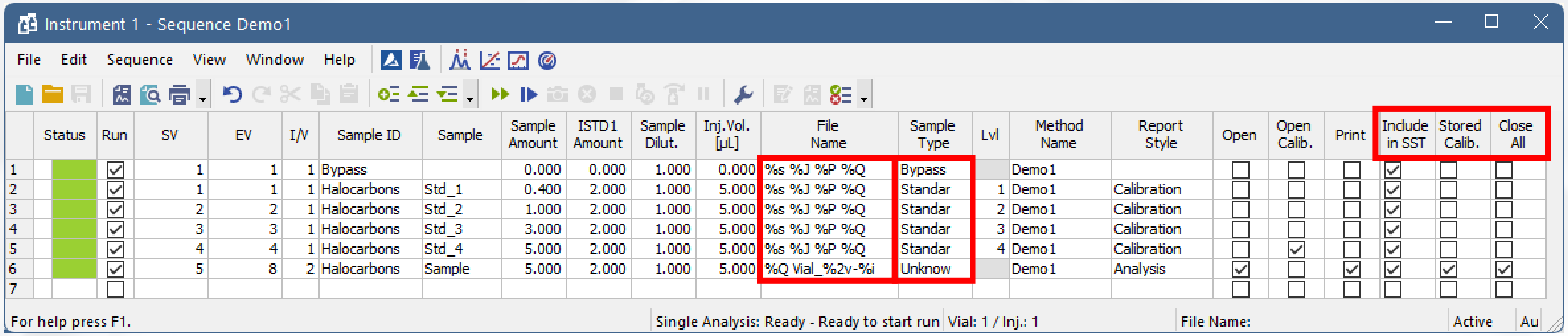
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1	🟧	☑	1	1	1	Halocarbons	Std_1	0.400	2.000	1.000	5.000	%Q	Stan	1	Demo1	Calibration	☐	☐	☐
2	🟩	☑	2	2	1	Halocarbons	Std_2	1.000	2.000	1.000	5.000	%Q	Stan	2	Demo1	Calibration	☐	☐	☐
3	🟩	☑	3	3	1	Halocarbons	Std_3	3.000	2.000	1.000	5.000	%Q	Stan	3	Demo1	Calibration	☐	☐	☐
4	🟩	☑	4	4	1	Halocarbons	Std_4	5.000	2.000	1.000	5.000	%Q	Stan	4	Demo1	Calibration	☐	☑	☐
5	🟩	☑	5	8	2	Halocarbons	Sample	5.000	2.000	1.000	5.000	%Q Vial_...	Unkn		Demo1	Analysis	☑	☐	☐
6		☐															☐	☐	☐

For help press F1. | 0.04 min - Running - Acquisition running | Vial: 1 / Inj.: 1 | File Name: Std_1 | Active | Aut

SEQUENCE WINDOW

BASIC FUNCTIONS

- Useful **file name variables**: %s = sequence, %J = Method, %P = project, %Q = Sample
- **Bypass** sample type = 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
- **Close All** – close all currently opened chromatograms in overlay



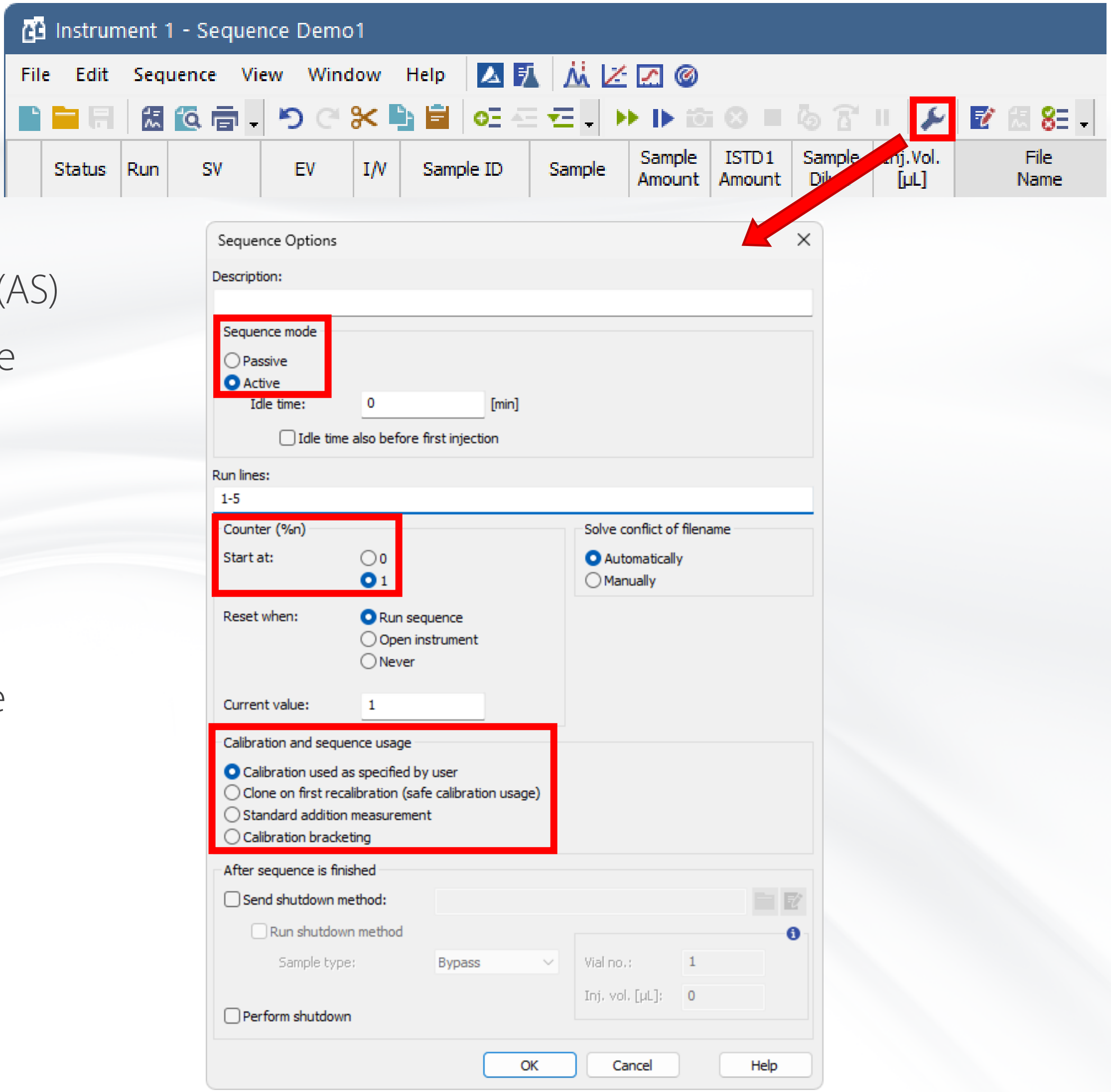
	Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj.Vol. [μL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print	Include in SST	Stored Calib.	Close All
1	🟩	☑	1	1	1	Bypass		0.000	0.000	1.000	0.000	%s %J %P %Q	Bypass		Demo1		☐	☐	☐	☑	☐	☐
2	🟩	☑	1	1	1	Halocarbons	Std_1	0.400	2.000	1.000	5.000	%s %J %P %Q	Standar	1	Demo1	Calibration	☐	☐	☐	☑	☐	☐
3	🟩	☑	2	2	1	Halocarbons	Std_2	1.000	2.000	1.000	5.000	%s %J %P %Q	Standar	2	Demo1	Calibration	☐	☐	☐	☑	☐	☐
4	🟩	☑	3	3	1	Halocarbons	Std_3	3.000	2.000	1.000	5.000	%s %J %P %Q	Standar	3	Demo1	Calibration	☐	☐	☐	☑	☐	☐
5	🟩	☑	4	4	1	Halocarbons	Std_4	5.000	2.000	1.000	5.000	%s %J %P %Q	Standar	4	Demo1	Calibration	☐	☑	☐	☑	☐	☐
6	🟩	☑	5	8	2	Halocarbons	Sample	5.000	2.000	1.000	5.000	%Q Vial_%2v-%i	Unknow		Demo1	Analysis	☑	☐	☑	☑	☑	☑
7		☐															☐	☐	☐	☐	☐	☐

For help press F1. | Single Analysis: Ready - Ready to start run | Vial: 1 / Inj.: 1 | File Name: | Active | Au

SEQUENCE WINDOW

SEQUENCE MODES AND OPTIONS

- **Passive sequence**: Clarity only expects the START signal, the time of analysis is set by the autosampler (AS)
- **Active sequence**: Clarity sends a READY signal to the AS and waits for the START signal
    - **AS control** in active sequence: AS injects according to SV, EX, I/V, and Inj. Volume in the Sequence Table
- Set the initial value for the **%n** variable
- Choose the **calibration mode** applied for the whole sequence



Description:

Sequence mode
○ Passive
● Active
Idle time: 0 [min]
☐ Idle time also before first injection

Run lines: 1-5

Counter (%n)
Start at: ○ 0 ● 1
Reset when: ● Run sequence ○ Open instrument ○ Never
Current value: 1

Solve conflict of filename
● Automatically
○ Manually

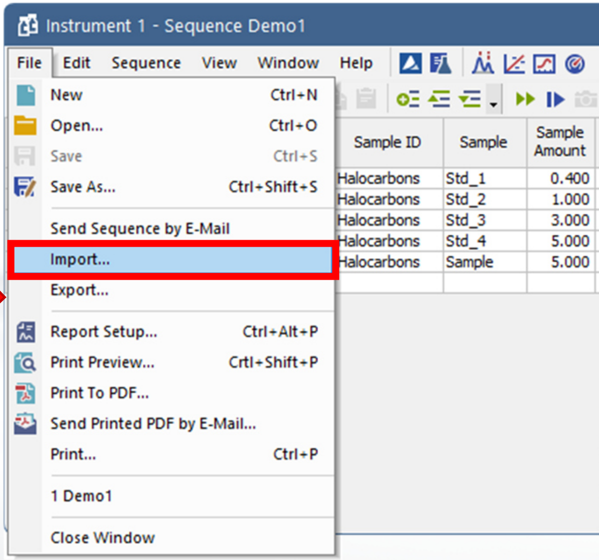
Calibration and sequence usage
● Calibration used as specified by user
○ Clone on first recalibration (safe calibration usage)
○ Standard addition measurement
○ Calibration bracketing

After sequence is finished
☐ Send shutdown method:
☐ Run shutdown method
Sample type: Bypass
Vial no.: 1
Inj. vol. [µL]: 0
☐ Perform shutdown

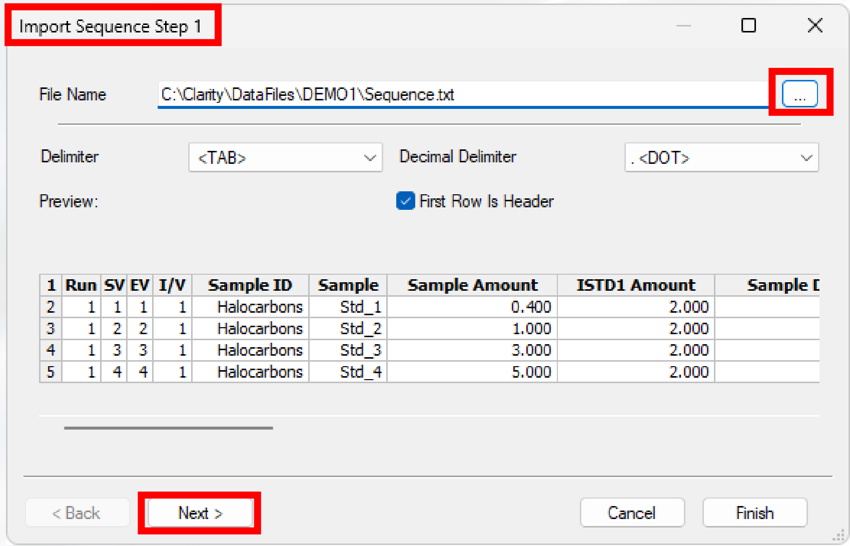
SEQUENCE WINDOW

IMPORT

- Import Sequence Step 1 dialog: select files to import
- Import Sequence Step 2 dialog: assign the respective fields to be imported
    - the Start Vial (SV) and File Name (both in bold) are mandatory



Sample ID	Sample	Sample Amount
Halocarbons	Std_1	0.400
Halocarbons	Std_2	1.000
Halocarbons	Std_3	3.000
Halocarbons	Std_4	5.000
Halocarbons	Sample	5.000



File Name C:\Clarity\DataFiles\DEMO1\Sequence.txt

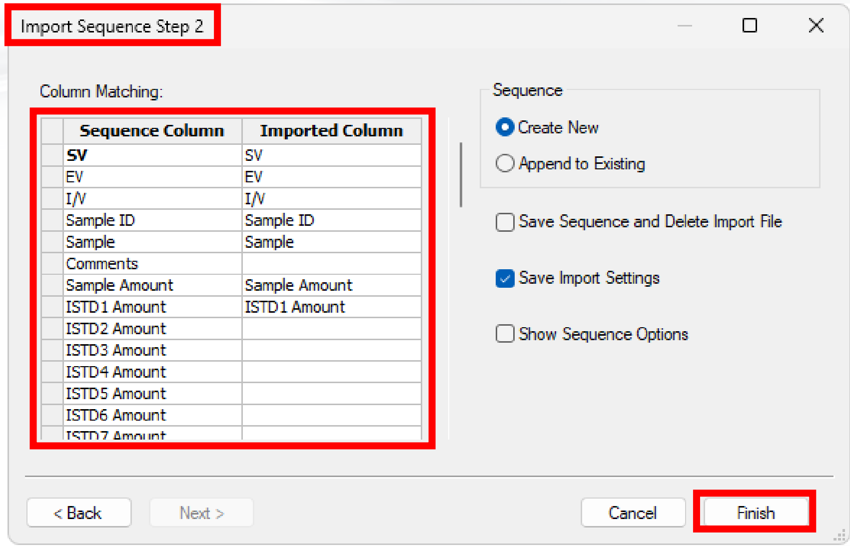
Delimiter <TAB>

Decimal Delimiter . <DOT>

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	



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	
ISTD7 Amount	

Sequence

● Create New

○ Append to Existing

☐ Save Sequence and Delete Import File

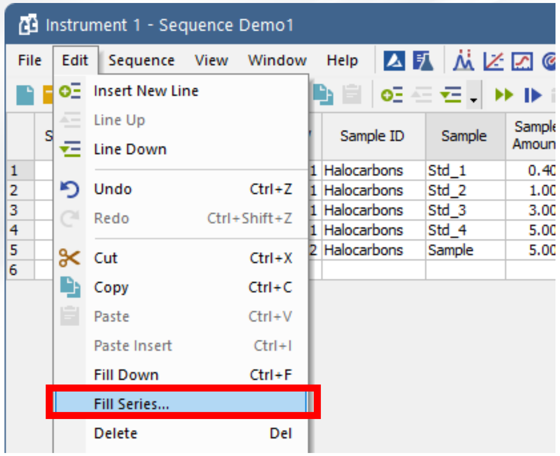
☑ Save Import Settings

☐ Show Sequence Options

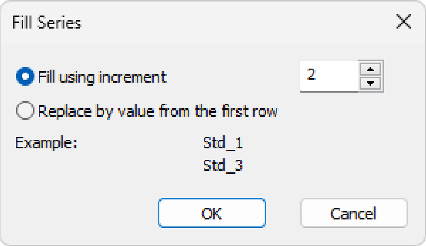
SEQUENCE WINDOW

FILL SERIES AND FILL DOWN

- Available in Sequence and Calibration
- Select a cell to be used for filling (numeric inputs, text inputs with numeric counters)
- Fill down (Ctrl+F):
    - Fill the cells below with the parameter in the selected cell
- Fill series:
    - Open the Fill Series dialog and specify the fill/replace parameters



	Sample ID	Sample	Sample Amoun
1	Halocarbons	Std_1	0.4
2	Halocarbons	Std_2	1.0
3	Halocarbons	Std_3	3.0
4	Halocarbons	Std_4	5.0
5	Halocarbons	Sample	5.0
6			



● Fill using increment 2

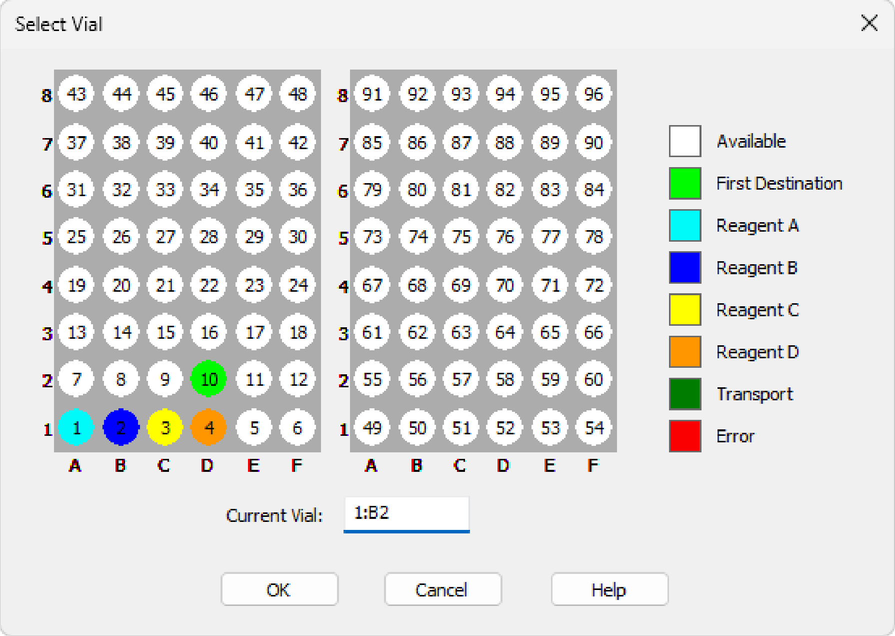
○ Replace by value from the first row

Example: Std_1
Std_3

SEQUENCE WITH AUTOSAMPLERS

SELECT VIAL

- The dialog with a graphic interface can be opened from Single Analysis/Sequence or viewed in Method Setup
- Convenient for working with **autosamplers** (available only in some AS)
- For controlled autosamplers, the **vial number** and **injection volume** are set in this dialog
- Allows **mid-run modifications** for not yet processed samples



	A	B	C	D	E	F
8	43	44	45	46	47	48
7	37	38	39	40	41	42
6	31	32	33	34	35	36
5	25	26	27	28	29	30
4	19	20	21	22	23	24
3	13	14	15	16	17	18
2	7	8	9	10	11	12
1	1	2	3	4	5	6

	A	B	C	D	E	F
8	91	92	93	94	95	96
7	85	86	87	88	89	90
6	79	80	81	82	83	84
5	73	74	75	76	77	78
4	67	68	69	70	71	72
3	61	62	63	64	65	66
2	55	56	57	58	59	60
1	49	50	51	52	53	54

☐ Available
🟩 First Destination
🟦 Reagent A
🟦 Reagent B
🟨 Reagent C
🟧 Reagent D
🟩 Transport
🟥 Error

Current Vial: 1:B2

23.0331

Clarity™

ADVANCED CHROMATOGRAPHY SOFTWARE

SHORT BREAK