Table of Contents

Batch Processing (Pro edition only)

MagicPlot Batch Processing allows to automatically process multiple similar data in the same way without programming (scripting) and recording of macro. One only have to ordinarily process the first data set manually and then use it as a template for processing of the rest data sets. Batch Processing includes the processing of data itself and semiautomatic fitting of the series of similar data.

Video Tutorial

Here is short video tutorial about batch processing: http://www.youtube.com/watch?v=L7RRraY6Dkc
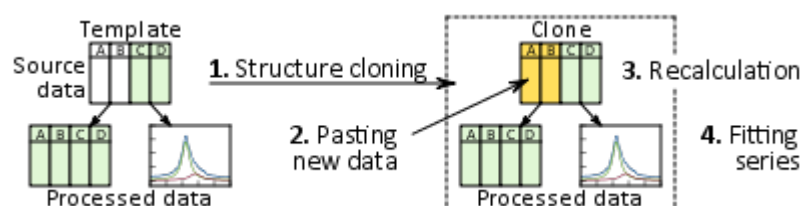
Introduction

Batch Processing idea is based on creating a copy of project components (Tables, Figures, Fit Plots) with formula links between them, pasting new data into the copy of source Table and recalculation of depending data using formulas.

The Table which contains the imported data from the first manually processed data set is called Template Table.

For each file MagicPlot will:

1. Create copies of Template Table and selected related components,
2. Paste new data to the leftmost columns of the copy of Template Table,
3. Recalculate all depending data in copies.

Fitting of series dialog will be opened after batch processing. This tool allows you to fit multiple data with the same model.

Capabilities

Batch Processing tool supports all MagicPlot data processing and visualization techniques:

- Calculating Table column with specified formula,
- Fourier transform,
- Integration/differentiation,
- Histogram calculation,

- [Creating of Figures and Fit Plots](),
- [Nonlinear curve fitting]().

These features are not supported by Batch Processing tool:

- Changing the sequence of columns with imported source data (inserting columns left, deleting and moving these columns),
- Table sorting.

Batch Processing Steps

It is supposed that you have a number of text (ASCII) files with similarly formatted source data to be processed.
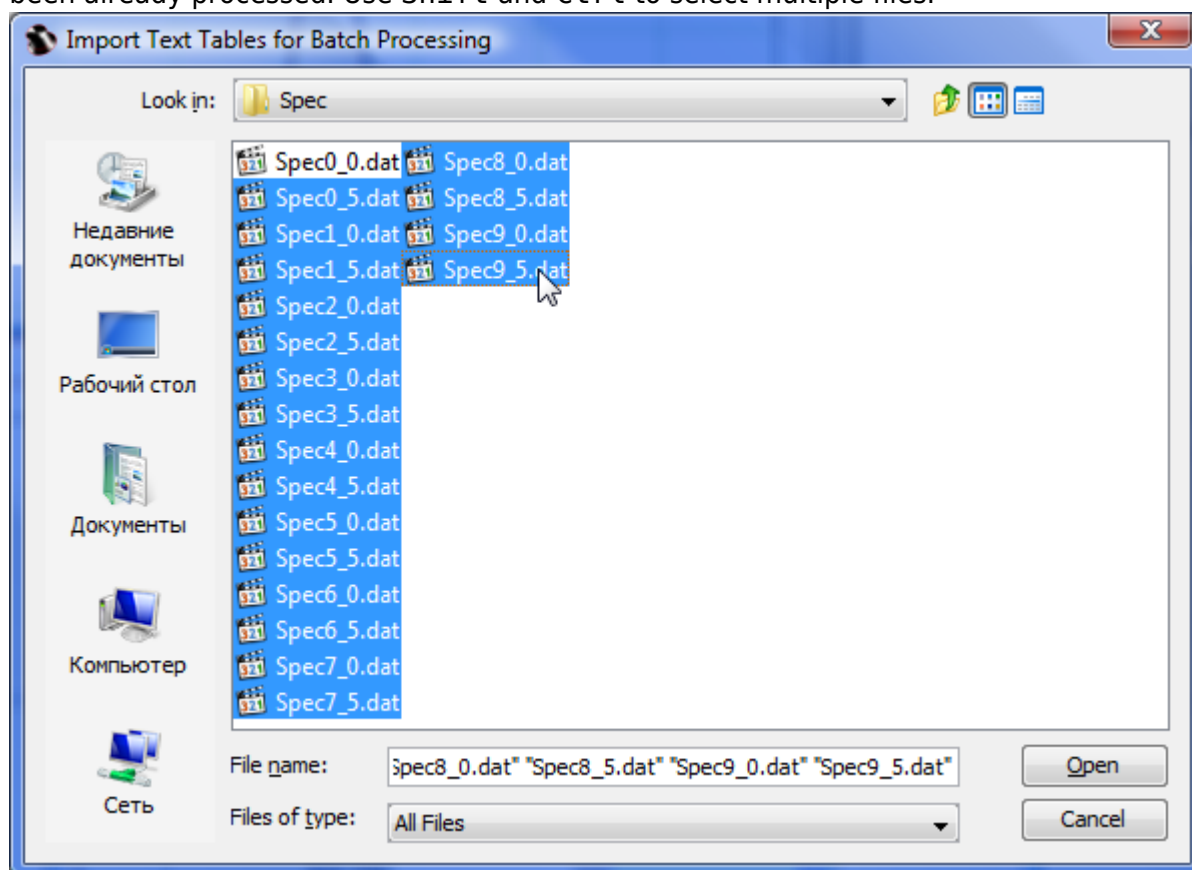
The overall processing steps are:

1. Import the first text file from series (`Project → Import Text Table…` menu item) and process it. You can add new columns with formulas, calculate some derivative data (histograms, FFT, etc.), create Figures and Fit Plots with one simple restriction:
   Do not change the sequence of leftmost columns with imported source data: do not insert columns left, delete and move these columns.
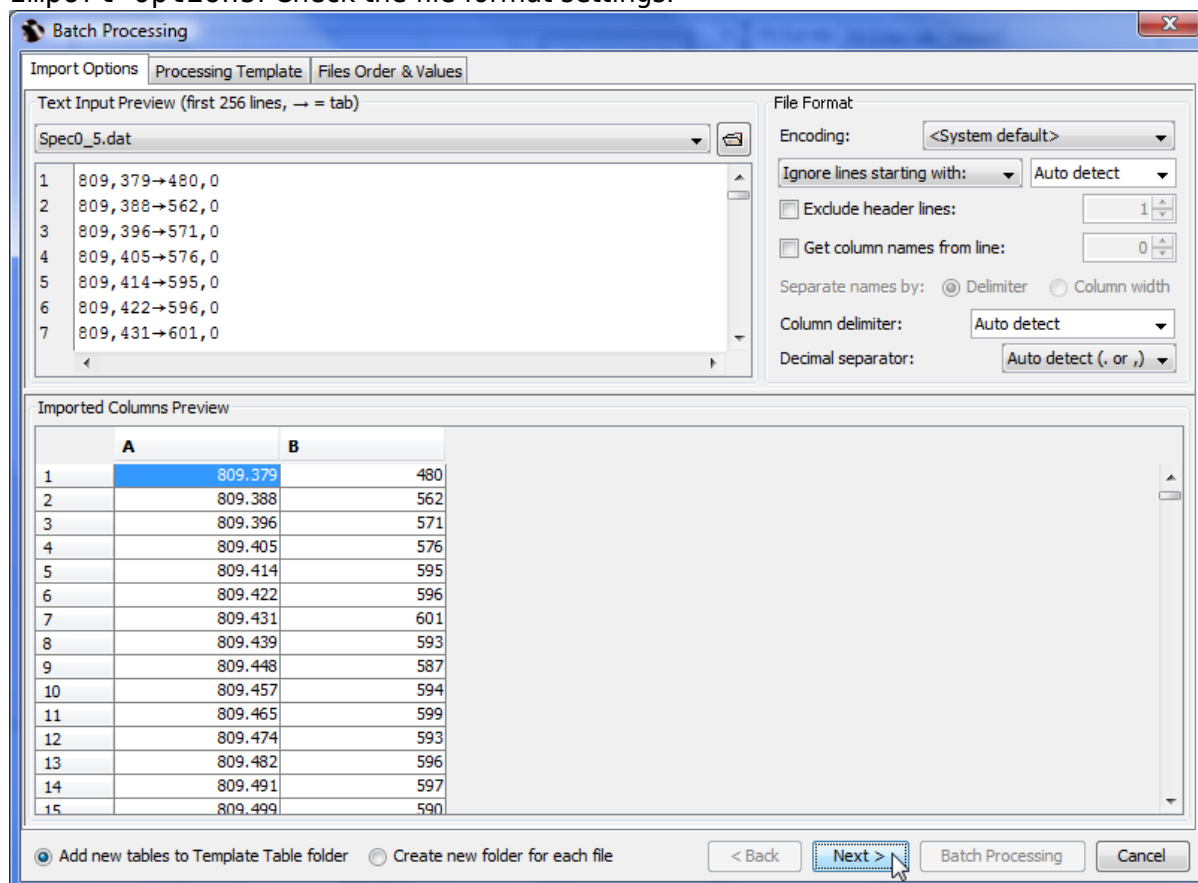   **Table sorting is also not supported in Batch Processing.**
   Create Fit Plot(s) and fit the first data in series if you want to fit series of data.
2. Run Batch Processing by selecting `Project → Import with Batch Processing…` menu item. In the opened file dialog select all rest files in the series except the first file which has been already processed. Use `Shift` and `Ctrl` to select multiple files.
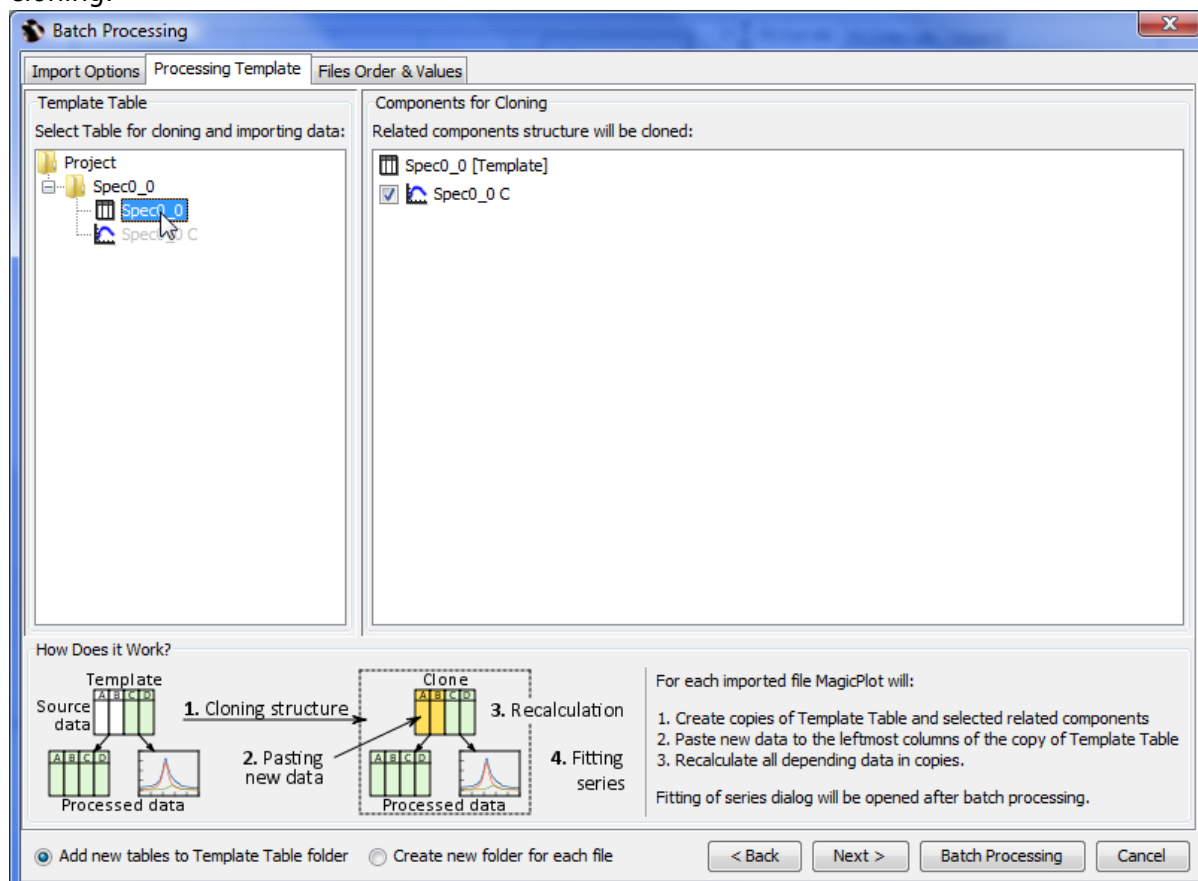
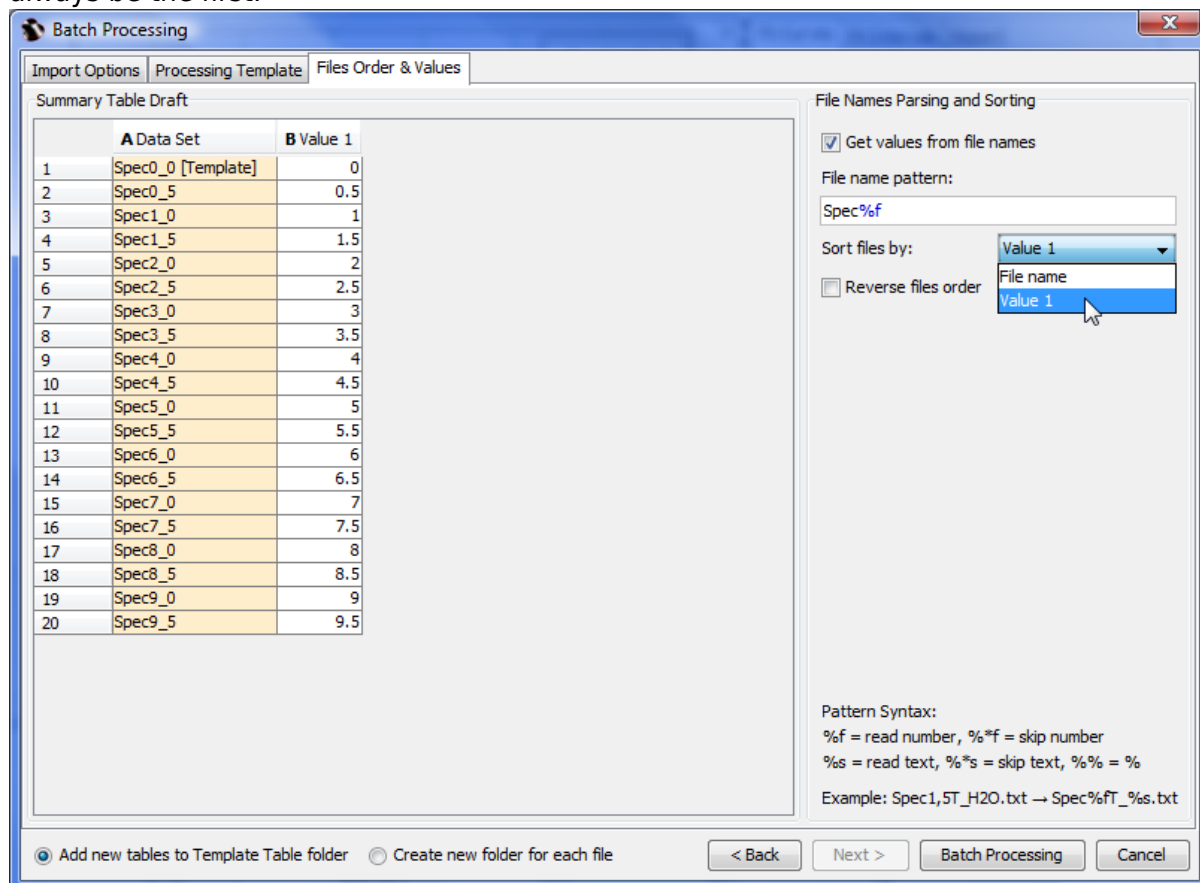3. In 3 tabs of `Batch Processing` dialog:
    1. `Import Options`: Check the file format settings.

    2. `Processing Template`: Specify the Table with data from the first file (already processed) as Template Table. The program will automatically show the derivative components with related data. You can also deselect some components to prevent cloning.

3. `Files Order & Values`: Set up the file names parsing to get some values to include into summary table. Select the files sorting. Note that the already processed file will always be the first.
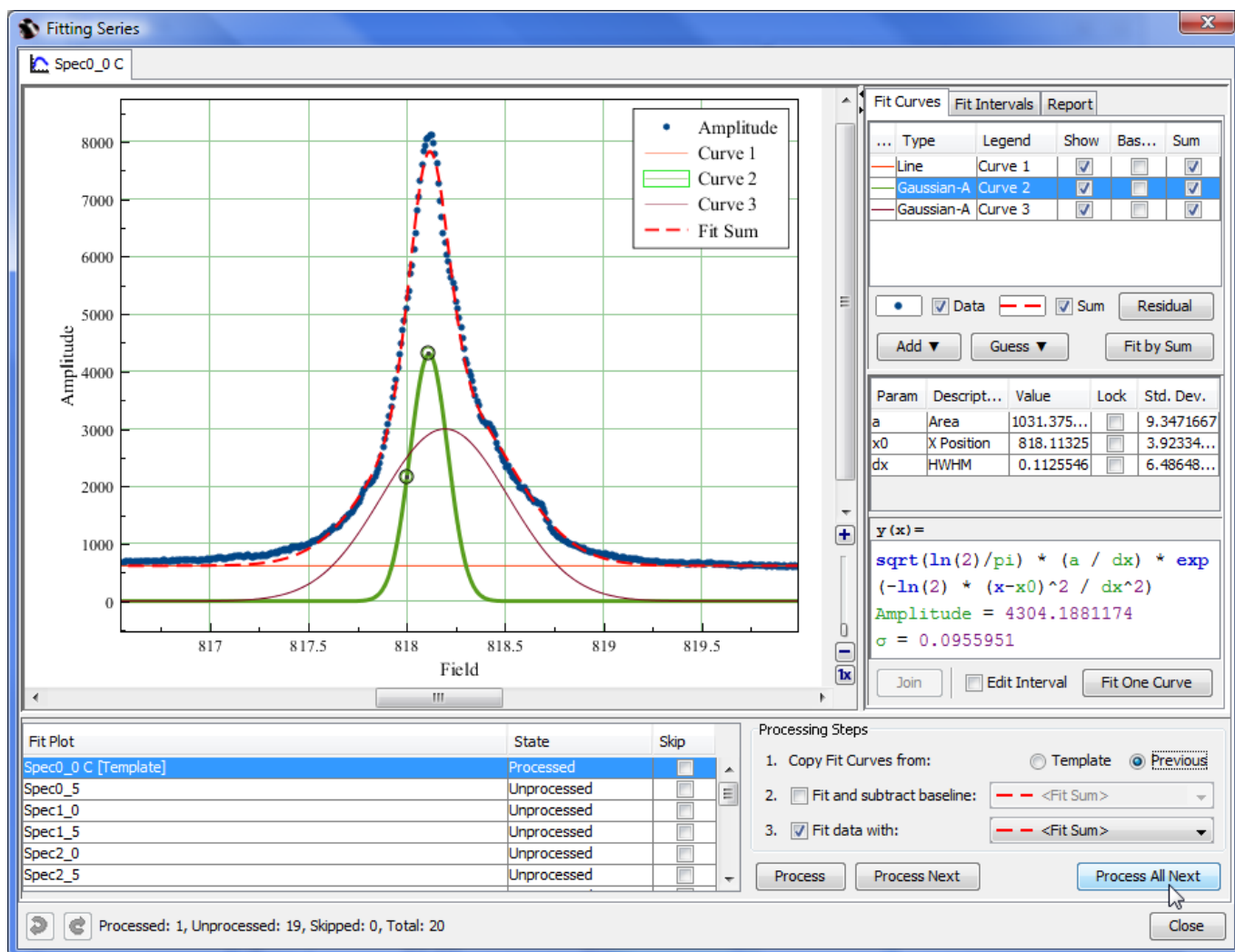

4. Click `Batch Processing` button to start processing. MagicPlot will create a copies of Template Table and all derivative components and paste new data in the leftmost columns.
5. The Fitting Series dialog will be opened if some Fit Plots were processed.

Fitting Series

The Fitting Series dialog will be opened after the batch processing finishes if some Fit Plots were created during the processing. If more than one Fit Plot was created for Template (and for each data set also), multiple tabs with Fit Plots will be shown in the window. Each tab will show one Fitting Series.

The Fitting Series dialog window is a standard Fit Plot panel with the list if data sets and options for the fitting series added on the bottom. Each data set will be processed in the same way as shown in the window:

1. The fit curves will be copied from the template plot (first in list) or from the (already fitted) previous plot depending on radio button selected (see more information below).
2. The baseline will be fitted with curve (selected in drop box) and subtracted from the experimental data.
3. The data will be fitted with selected curve or sum curve (selected in drop box).

Curves and Initial Values of Parameters: from the Template or from Previous Data Set?

Please pay attention on the source curves alternative: from the template or from the previous data set. This setting manage which curves and initial values of parameters will be used for nonlinear fitting of each data set. The recommendations are the following:

- Select 'Previous' if your data in data set changes 'evolutionary': the values of parameters (ex. peak positions) are changed progressively from one plot to another. This variant appears when you examine the dependency of your data on some parameter. Example: you heat the sample step by step and measure the spectrum; the temperature rises from one spectrum to another and peaks are moved. Each plot is more similar to the previous one then to the first one (the template).
- Select 'Template' if all of your data sets are independent and no 'evolution' process can be seen between plots. Each plot is more similar to the first one (the template) then to the previous one.

Automatic and Step by Step Modes

You have 3 alternative buttons to process:

- Process – processes the currently selected Fit Plot: The curves are copied from the previous or

the first Fit Plot and fitting is performed. All existing curves will be removed from current Fit Plot before coping curves from previous/first Fit Plot.

- Process Next – opens and processes the next Fit Plot.
- Process All Next – automatically processes all the Fit Plots next to the currently selected Fit Plot. This option is equal to the manually pressing 'Process Nest' button until all Fit Plots will be processed.

Semi-Automatic Mode

When using step-by-step batch processing ('Process / Process Next buttons) you can change the fit for the currently selected plot. You can change the initial values of the parameters (move peaks manually), add or remove peaks. Don't forget to launch the fitting after the manual changing of the curve list or the parameters values. ==== Summary Table ==== Summary Table will be created after finishing fitting series. This table contains the values of all fit parameters and standard errors for all processed data sets. You can use this data to create a Figure or Fit Plot or export it. By default the values in Summary Table will be updated if the values of fit parameters on Fit Plots changes.

	A Data Set	B Value 1	C Curve 1.a	D ±Δ Curve 1.a	E Curve 1.b	F ±Δ Curve 1.b	G Curve 2.a
1	Spec0_0 [Template]	0	-0.6417315	0.2291674	1141.2610974	187.4428964	1031.37
2	Spec0_5	0.5	-0.2150654	0.1873521	785.2007576	153.2365908	745.36
3	Spec1_0	1	-0.3654919	0.1136925	903.7396066	92.9882536	649.95
4	Spec1_5	1.5	-0.4025649	0.2537475	932.6400411	207.5412417	501.46
5	Spec2_0	2	-0.3366649	0.2943521	881.3126685	240.760401	434.32
6	Spec2_5	2.5	-0.2094106	0.2858062	779.2973761	233.7781807	329.65
7	Spec3_0	3	-0.2377343	0.2905013	803.2012531	237.6244468	604.66
8	Spec3_5	3.5	0.1538196	0.3441019	487.4428375	281.4758354	1275.3
9	Spec4_0	4	-0.3347863	0.4337912	886.1718936	354.856993	1478.06
10	Spec4_5	4.5	0.0883859	0.5214879	536.0243193	426.6157848	1676.18
11	Spec5_0	5	0.0463876	0.5026314	568.9729216	411.2058363	1582.66
12	Spec5_5	5.5	-0.1446354	0.5256476	726.2031958	430.0505361	1607.
13	Spec6_0	6	-0.1292856	0.5151819	714.3564312	421.5007319	1506.68
14	Spec6_5	6.5	-0.466563	0.4711707	992.4459904	385.4985279	1029.48
15	Spec7_0	7	-0.2411057	0.408633	806.3679948	334.3401114	780.45
16	Spec7_5	7.5	-0.6643598	0.2960808	1161.5518378	242.2302287	1588.23
17	Spec8_0	8	-1.0487862	0.3121694	1478.5074471	255.397587	1250.96

=== Reopening Fitting Series Dialog === You can open Fit Series dialog using Fit Series Summary → Open Fitting Series Dialog...'' in summary table.

	A Data Set	B Value 1	C Curve 1.a	D ±Δ Curve 1.a	E Curve 1.b	F ±Δ Curve 1.b	G Curve 2.a
1	Spec0_0 [Template]	0					1031.37
2	Spec0_5	0.5	f(x) Fit Series Summary ▶	Open Fitting Series Dialog... Ctrl+F2			745.36
3	Spec1_0	1					649.95
4	Spec1_5	1.5	Create Figure ▶	Recalculate Ctrl+Enter			501.46
5	Spec2_0	2	Add to Selected Axes ▶	✓ Auto Recalculate			434.32
6	Spec2_5	2.5					329.65
7	Spec3_0	3	Create Fit Plot ▶	Output Data ▶			604.66
8	Spec3_5	3.5					1275.3
9	Spec4_0	4	Cut Ctrl+X	Remove Formula			1478.06
10	Spec4_5	4.5	Copy Ctrl+C				1676.18
11	Spec5_0	5			568.9729216	411.2058363	1582.66
12	Spec5_5	5.5	Paste Ctrl+V		726.2031958	430.0505361	1607.

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