Table of Contents

Help topics on the Next MagicPlot Release

These topics will be added in MagicPlot Help when next version will be released.

- in Preview Image

Upload new screenshot

- in Export Curves as Table

Upload new screenshot of Table from curves

- in Nonlinear Curve Fitting: Fit Plot

Extract 'Specifying Custom Fit Curve (Fit Formula) (Pro edition only)' Create subsection 'Nonlinear Curve Fitting' in contents

---

- in Guessing Peaks

Guess Peaks (Pro only)

MagicPlot can approximately locate peaks in spectrum. To locate peaks click on `Guess` button in `Fit Curves` tab of Fit Plot. Peak guessing is performed by looking for local minimums of second derivative of data-baseline.

While `Guess Peaks` window is open you will see the preview of guessed peaks on Fit Plot. This preview will be updated every time you change the parameters in the window.

Smoothing of Data and 2nd Derivative

Smoothing is applied in order to filter narrow peaks which can be guessed from noise. MagicPlot peak guess tool is capable to smooth both data and second derivative before finding local minimums. Smoothing if used only to find peaks and does not affect the data on Fit Plot.

Savitzky–Golay method is used for smoothing. This algorithm performs a local polynomial regression of specified degree on specified number of points. Bigger points number leads to better smoothing.

The Number of Peaks

MagicPlot sorts founded peaks by amplitude and guess only the specified number of greatest peaks. You can change the number of guessed peaks with slider or by entering value in the text field with spinner.

- in Using Spline for Baseline Subtraction

Using Spline for Baseline Subtraction (Pro only)

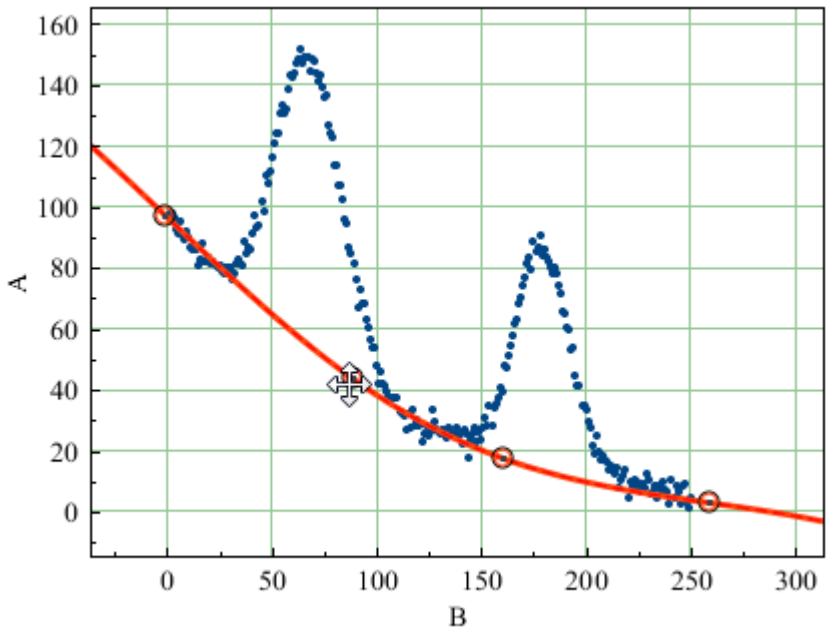
You can use cubic spline to fit and subtract baseline on Fit Plot. To create spline curve click on Add button in `Fit Curves` tab of Fit Plot.

Don't use splines to subtract baselines which can be good fitted by line curve (line or constant baseline). You can subtract wide peaks by mistake using spline.

Editing Spline

Created spline has 3 anchor points by default. You can move, add and remove anchor points:

- Move anchor point with mouse
- Double click on spline curve to add new anchor point
- Double click on anchor point to remove it

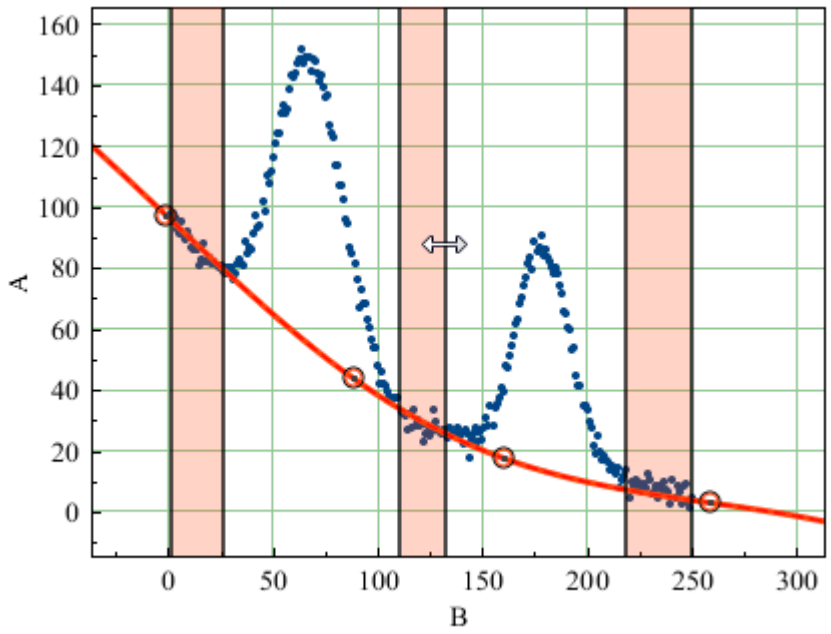


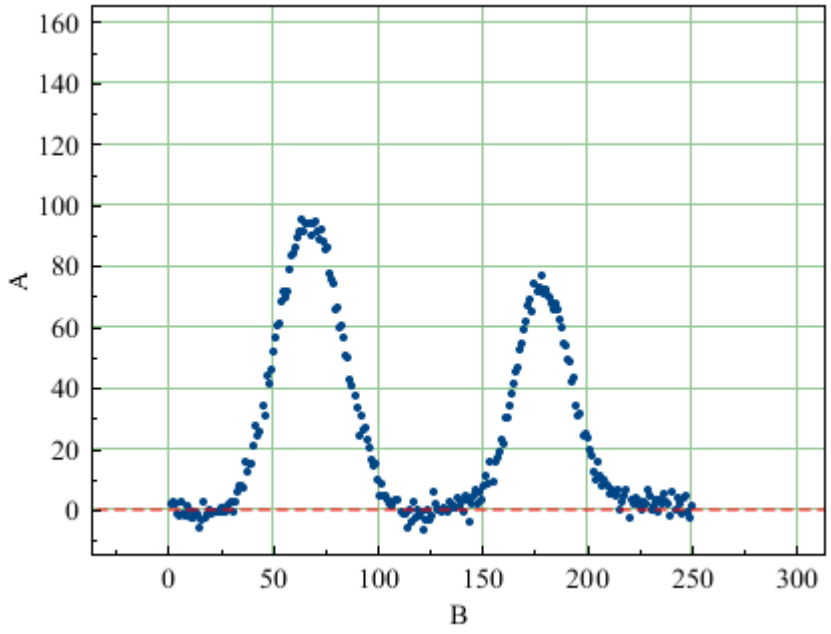
Fitting with Spline

Spline anchor point (*x*, *y*) coordinates are treated as fit parameters so you can perform fitting by spline. Note that the anchor point coordinates will be varied but the number of point will remain. You also can lock some parameters (usually *x* coordinates) by setting `Lock` check boxes in parameters table.

It is recommended to set appropriate fit intervals which contains only baseline without peaks. In such case `Fit One Curve` button is more usable than `Fit by Sum` button because the individual interval for current curve will be used and the interval from `Fit Interval` tab (which is used to fit by sum of curves) is ignored. Select spline curve and check `Set Interval` check box in the bottom of the panel to edit spline interval, then click on `Fit One Curve` button.

Set `Baseline` check box in spline row in curves table to subtract spline from data.





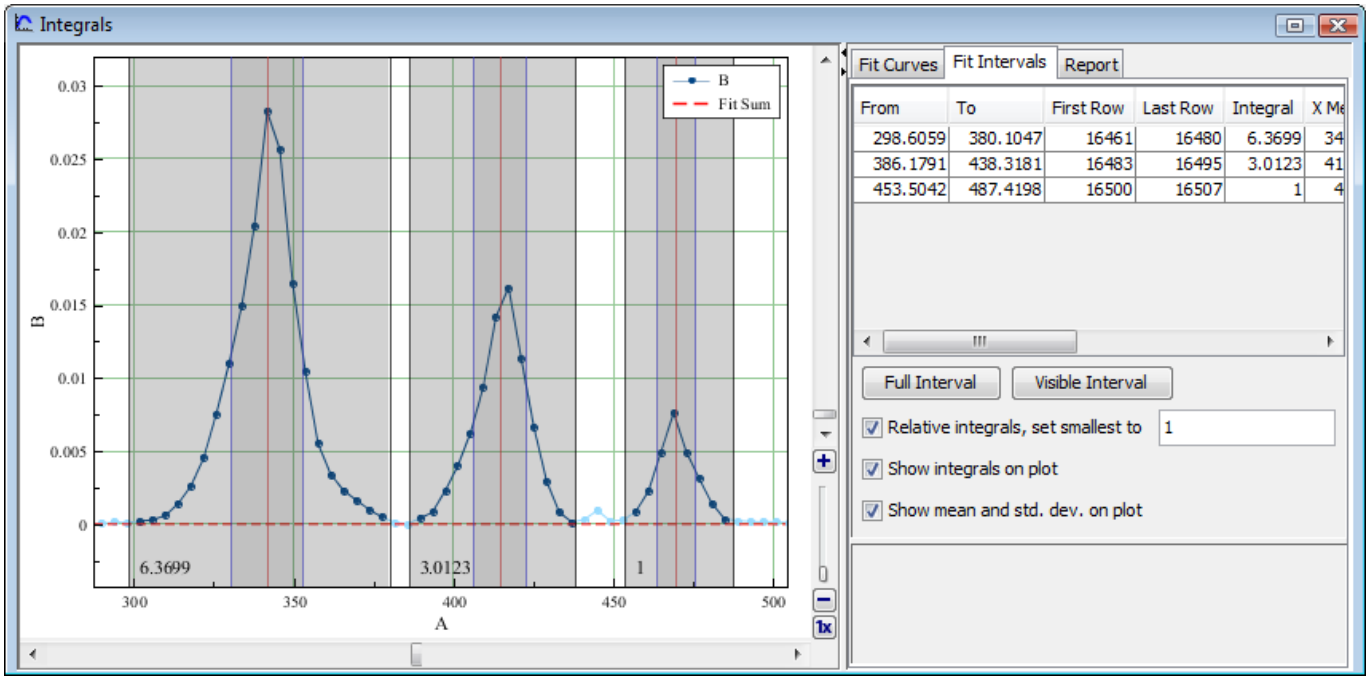
- in Calculating Integrals and Statistics on Intervals using Fit Plot

Integrals and Statistics on Intervals

Setting intervals in `Fit interval` tab of Fit Plot is initially intended for setting data range which is used for fitting by sum of fit curves. However this tab can also be used to calculate integrals and statistics on these intervals (Statistics is only available in Pro edition). Data-Baseline is used to calculate the results.

MagicPlot is capable to integrate data on selected intervals and to calculate peak moments (x mean, variance, skewness, kurtosis). Spectrum line is treated as probability distribution curve: *x* values are treated as 'independent variable' and *y* values are treated as 'probability'. Standard statistical formulas are used to calculate moments.

Statistical data and integrals are automatically updated if *x* or *y* data is changed or intervals are changed.



All statistical data is summarized in the intervals table:

From	To	First Row	Last Row	Integral	X Mean	Variance	Std.dev.	Skewness	Kurtosis	Y Sum	Points
298.6059	380.1047	16461	16480	6.3699	341.6323	128.0854	11.3175	8.7703e-4	0.6547	0.1588	20
386.1791	438.3181	16483	16495	3.0123	414.6365	68.0536	8.2495	-0.3499	0.0449	0.0752	13
453.5042	487.4198	16500	16507	1	469.668	35.0647	5.9215	0.1509	-0.2173	0.0255	8

Managing Intervals

Move interval borders with mouse. Double click on interval to split it at desired position. Right click

opens context menu from which new intervals can be created on free space and existing intervals can be deleted or split.

Relative Integrals Calculation

MagicPlot is capable of calculation relative integrals to compare the relative intensity of spectrum lines. To compute relative integrals set `Relative integrals` check box. MagicPlot designate the smallest integral as 1 but you can enter a custom value. If you want not the smallest integral to be the reference point enter 1 firstly and than enter the value of desired integral relative to 1 to this field so that other integrals will be calculated relative to this new value.

Formulas

Property	Formula
Integral	Calculated using Trapezoidal rule
X Mean (expected value)	$\mu = \nu_1$
Variance	$\sigma^2 = \mu_2$
Standard deviation	$\sigma = \sqrt{\mu_2}$
Skewness	$\gamma_1 = \frac{\mu_3}{\mu_2^3}$
Kurtosis	$\gamma_2 = \frac{\sigma^4}{\sum_k \sigma_k^4} - 3$
Y Sum	$s = \sum_k y_k$

Intermediate values are calculated as follows:

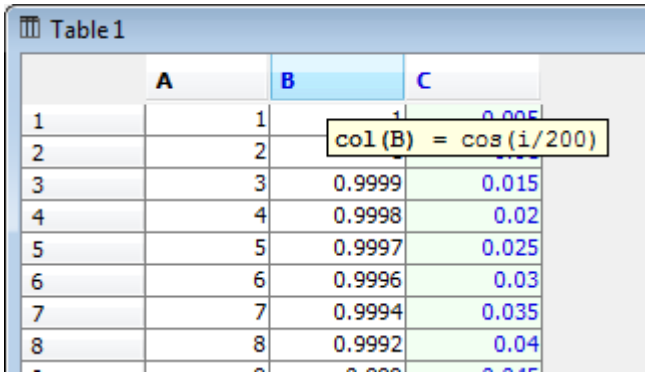
Property	Formula
Raw moments	$\nu_n = \frac{1}{s} \sum_k y_k x_k^n$,~ n = 1...4
Normalization coefficient	$s = \sum_k y_k$
Central moments	$\mu_3 = \nu_3 - 3\nu_1\nu_2 + 2\nu_1^3$

- in Table Editing

Upload new menu screenshot

Displaying Column Formulas in Table

MagicPlot indicates columns for which formulas or other evaluators (FFT, integral, etc.) are set with blue header color. You can see the formula in column header tool tip.



On the screenshot above:

- Column A has no formula
- Column B has formula, auto recalculation is off
- Column C has formula, auto recalculation is on, so this column is not editable

Fit Column Widths

To fit the width of one column double click on right separator line in table header. To fit selected columns widths double click one of column separators in table header.

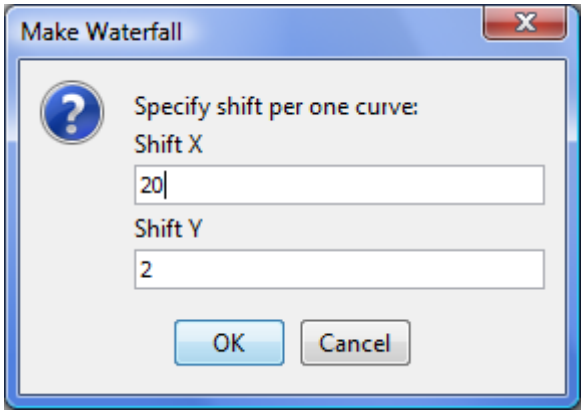
- in transform xy

Transform X or Y Column (Pro only)

You can quick transform X or Y data on Fit Plot by using `Transform X/Y` items in `Processing` menu. This menu items open set column formula dialog for table column which is used as X or Y. Note that this transformation affects the table with plot data.

- in Shifting Curves on Figure and Creating 2D Waterfall

`Make Waterfall` menu item opens waterfall window in which you can specify shift increment. MagicPlot tries to guess beautiful shift values on basis of the number of curves and current scale.



- in Fast Fourier Transform (FFT)

Upload new screenshot, update formulas

- in MagicPlot Calculator

Update screenshot.

MagicPlot can be minimized to task bar while Calculator window can be still on top

---

- in Predefined Fit Curves Equations

Fit Curves Types

This is the table of predefined fit curves.

Name	Formula	Additional Properties
Line	$y=ax+b$	
Parabola	$y=ax^2+bx+c$	Vertex:
Gaussian	$y=a\exp\left(-ln2\left(\frac{x-x_0}{dx}\right)^2\right)$	Area: $S=\frac{\sqrt{\pi}}{\sqrt{ln2}}adx$ Standard deviation: $\sigma=\frac{dx}{2\sqrt{ln2}}$
Gaussian-A (normalized)	$y=\sqrt{\frac{ln2}{\pi}}\frac{a}{dx}\exp\left(-ln2\left(\frac{x-x_0}{dx}\right)^2\right)$	Amplitude: $A=\sqrt{\frac{ln2}{\pi}}\frac{a}{dx}$ Standard deviation: $\sigma=\frac{dx}{2\sqrt{ln2}}$
Lorentzian	$y=\frac{a}{1+\left(\frac{x-x_0}{dx}\right)^2}$	Area: $S=\pi adx$ Amplitude: $A=\frac{a}{\pi dx}$
Lorentzian-A (normalized)	$y=\frac{1}{\pi dx}\frac{a}{1+\left(\frac{x-x_0}{dx}\right)^2}$	Area (second integral): $S=a$ Standard deviation: $\sigma=\frac{dx}{2}\sqrt{\frac{\pi^2}{ln2}-2}$ Peak-to-peak horizontal: $p_x=2dx\sqrt{\frac{ln2}{\pi^2}}$ Peak-to-peak vertical: $p_y=\sqrt{\frac{ln2}{\pi^2}}\frac{a}{dx}$
Gauss Derivative	$y=-2\ln 2\frac{a(x-x_0)}{dx^2}\exp\left(-ln2\left(\frac{x-x_0}{dx}\right)^2\right)$	

Name	Formula	Additional Properties
Lorentz Derivative	$$y=-2a\frac{\left(x-x_0\right)}{dx^2}\left(1+\left(\frac{x-x_0}{dx}\right)^2\right)^{-2}$$	Area (second integral): $S=\pi ab$ Peak-to-peak horizontal: $p_x=\frac{2}{\sqrt{3}}dx$ Peak-to-peak vertical: $p_y=\frac{3\sqrt{3}}{4}\frac{a}{dx}$