PeakFit™

Version 4.12

Automated Peak Separation and Analysis

PeakFit is a nonlinear peak separation and analysis software package that facilitates accurate peak analysis and conclusive results. It can locate, separate and measure up to 100 peaks at a time. It also includes highly advanced data smoothing and manipulation techniques to precisely process very noisy data (FFT, Gaussian convolution, Savitzky-Golay, and Loess algorithms). PeakFit's automation also simplifies peak finding and fits up to 100 peaks to a data set at a time enabling users to more accurately and conveniently characterize peaks and find the best equation for their data. PeakFit also includes AI (artificial intelligence) experts at all key points to help users pick out the best values for percent smoothing and filtering levels. Graphical placement options in the software allow users to override PeakFit's automation at anytime.

Peakfit is the automatic choice for spectroscopy, chromatography or electrophoresis

For Spectroscopy

PeakFit lets you accurately detect, separate and quantify hidden peaks that standard instrumentation misses. PeakFit includes 18 different nonlinear spectral application line shapes, including the Gaussian, the Lorentzian and the Voigt as well as a Gaussian plus Compton Edge model for fitting Gamma Ray peaks. As a product of the curve fitting process, PeakFit reports amplitude (intensity), area, center and width data for each peak. Overall area is determined by integrating the peak equations in the entire model. PeakFit can even deconvolve your spectral instrument response so that you can analyze your data without the smearing that your instrument introduces.

For Electrophoresis

PeakFit gives you the ability to quickly and easily separate, locate and measure up to 100 peaks (bands), even if they overlap. With 82 nonlinear peak models to choose from, you're almost guaranteed to find the best equation for your data. The sophisticated array of baseline types lets you integrate only the significant portion of the bands in your data. The results of these measurements are then automatically recorded in a PeakFit- generated report, or they can be shown graphically. PeakFit with a hand scanner can often replace $10,000 electrophoresis instruments with better results!

For Chromatography

PeakFit includes 8 different built-in equations for asymmetric peaks typically found in chromatography data: the Exponentially-Modified Gaussian, the Haarhoff-Van der Linde, the NLC, the Giddings and even a Half-Gaussian Modified Gaussian (an experimental model similar to the EMG, but used to describe intra-column originated asymmetry). The peak area is computed directly as a parameter within each of these functions, ensuring accuracy and enabling computation of confidence limits. PeakFit reports column efficiency, resolution, first moment (center of mass), second moment, center (mode), peak width at base and half maximum, and asymmetry at base and 10% of maximum. PeakFit can even deconvolve your chromatographic detector response, so you can analyze your data without instrument-induced asymmetry. PeakFit also supports AIA data file input.

For Signal Component Analysis

Even though PeakFit is widely used by chemists, biologists, etc., many electrical engineers have found PeakFit's statistical nonlinear fitting techniques extremely useful for separating overlapping signals.
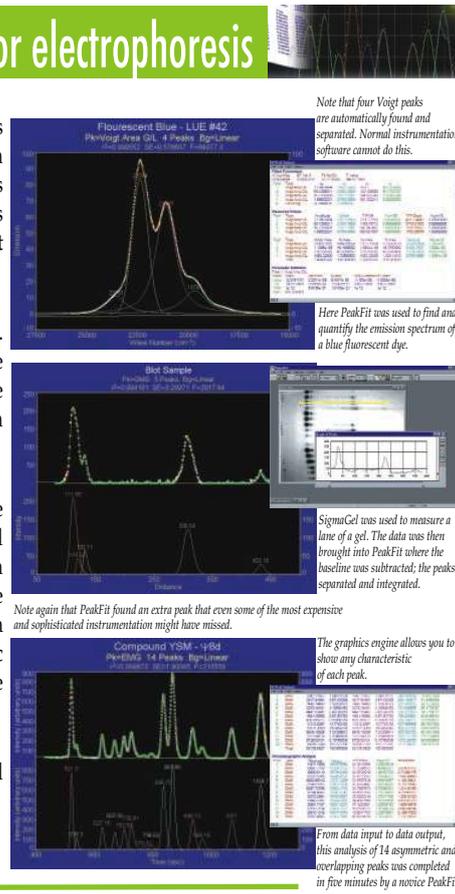
Note that four Voigt peaks are automatically found and separated. Normal instrumentation software cannot do this.

Here PeakFit was used to find and quantify the emission spectrum of a blue fluorescent dye.

SigmaGel was used to measure a lane of a gel. The data was then brought into PeakFit where the baseline was subtracted; the peaks separated and integrated.

Note again that PeakFit found an extra peak that even some of the most expensive and sophisticated instrumentation might have missed.

The graphics engine allows you to show any characteristic of each peak.

From data input to data output, this analysis of 14 asymmetric and overlapping peaks was completed in five minutes by a novice PeakFit user.

A True VOIGT Function...
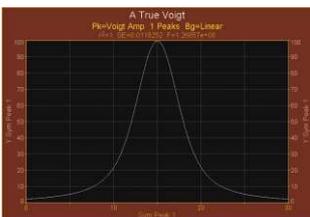
This pure voigt was created using PeakFit's data transform feature

In Spectroscopy, instrument and Doppler broadening effects create a Gaussian line shape, while natural and collision broadening cause a Lorentzian line shape. The Voigt function is a convolution of both the Gaussian and Lorentzian functions. Most analysis packages that offer a Voigt function use an approximation with very limited precision. PeakFit actually uses a closed-form solution to precisely calculate the function analytically. PeakFit has four different Voigt functions, so you can fit the parameters you're most interested in, including the individual widths of both the Gaussian and Lorentzian components, and the amplitude area of the Voigt function. PeakFit's precise calculation of the Voigt function is crucial to the accuracy of your analysis.
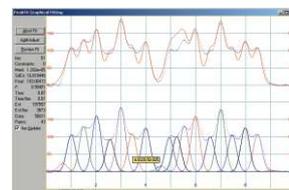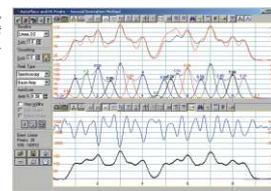
Peakfit's Automation makes it as easy as 1-2-3

PeakFit Automatically places peaks in three ways

With just a few clicks of the mouse, PeakFit's second derivative placement method finds 15 overlapping peaks.

PeakFit uses three procedures to automatically place hidden peaks; while each is a strong solution, one method may work better with some data sets than the others.

1. The Residuals procedure initially places peaks by finding local maxima in a smoothed data stream. Hidden peaks are then optionally added where peaks in the residuals occur.
2. The Second Derivative procedure searches for local minima within a smoothed second derivative data stream. These local minima often reveal hidden peaks.
3. The Deconvolution procedure uses a Gaussian response function with a Fourier deconvolution / filtering algorithm. A successfully deconvolved spectrum will consist of "sharpened" peaks of equivalent area. The goal is to enhance the hidden peaks so that each represents a local maximum.

Then with just one more click, PeakFit iterates until the fit is optimal.

Peakfit's state-of-the art-nonlinear curve fitting is essential for accurate peak analysis and conclusive findings

WHY SHOULD YOU USE NONLINEAR CURVE FITTING? - Nonlinear curve fitting is by far the most accurate way to reduce noise and quantify peaks. Many instruments come with software that only approximates the fitting process by simply integrating the raw data numerically. When there are shouldered or hidden peaks, a lot of noise, or a significant background signal, this can lead to the wrong results. For example, a spectroscopy data set may appear to have a peak with 'raw' amplitude of 4,000 units - but may have a shoulder peak that distorts the amplitude by 1,500 units. This would be a significant error. PeakFit helps you separate overlapping peaks by statistically fitting numerous peak functions to one data set, which can help you find even the most obscure patterns in your data. The background can be fit as a separate polynomial, exponential, logarithmic, hyperbolic or power model. This fitted baseline is then subtracted before peak characterization data (such as areas) are calculated, which gives much more accurate results. And, any noise (from electrophoretic gels or Raman spectra) that might bias raw data calculations is filtered simply by the nonlinear curve fitting process. Nonlinear curve fitting is essential for accurate peak analysis and accurate research.
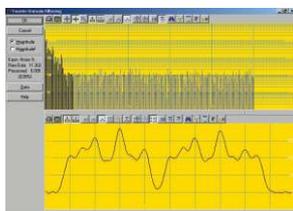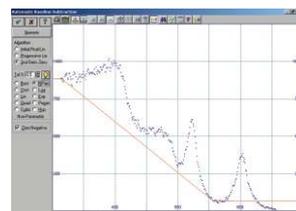

PeakFit's visual FFT filter allows you to easily see what frequencies should be zeroed.

PEAKFIT OFFERS SOPHISTICATED DATA MANIPULATION - With PeakFit's visual FFT filter, you can inspect your data stream in the Fourier domain and zero higher frequency points - and see your results immediately in the time-domain. This smoothing technique allows for superb noise reduction while maintaining the integrity of the original data stream. PeakFit also includes an automated FFT method as well as Gaussian convolution, the Savitzky-Golay method and the Loess algorithm for smoothing. AI Experts throughout the smoothing options and other parts of the program automatically help you set many adjustments. And, PeakFit even has a digital data enhancer, which helps analyze sparse data. Only PeakFit offers so many different methods of data manipulation.

HIGHLY ADVANCED BASELINE SUBTRACTION - In this example, PeakFit's non-parametric baseline fitting routine easily removes the complex background of a DNA electrophoresis sample. PeakFit can also subtract 8 other built-in baseline equations, or it can subtract any baseline you've developed and stored in a file.

PeakFit handles the complex backgrounds of gels with ease.

FULL GRAPHICAL PLACEMENT OF PEAKS - If PeakFit's auto-placement features fail on extremely complicated or noisy data, you can place and fit peaks graphically with only a few mouse clicks. Each placed function has "anchors" that adjust even the most highly complex functions, automatically changing that function's specific numeric parameters. PeakFit's graphical placement options handle even the most complex peaks as smoothly as Gaussians.

PUBLICATION-QUALITY GRAPHS AND DATA OUTPUT - Every publication-quality graph on this page has been created using PeakFit's built-in graphics engine - which now includes print preview and extensive file and clipboard export options. The numerical output is customizable so that you see only the content you want.

PEAKFIT SAVES YOU PRECIOUS RESEARCH TIME - For most data sets, PeakFit does all the work for you. What once took hours now takes minutes - with only a few clicks of the mouse! It's so easy that even a novice can learn how to use PeakFit in no time. And if you have extremely complex or noisy data sets, the sophistication and depth of PeakFit's data manipulation techniques is unequaled.

Nonlinear Peak Separation & Analysis for Spectroscopy, Chromatography & Electrophoresis

PeakFit separates and analyzes nonlinear peak data better, more accurately and more conveniently than your lab instrument - here's why:

- Advanced nonlinear curve fitting techniques separate overlapping peaks that standard instrumentation misses.
- Peak finding and fitting is fully automated! PeakFit has three different procedures to accurately characterize normal and hidden peaks.
- Graphically fit peaks yourself when you want to override PeakFit's automation.
- Highly advanced data smoothing and manipulation techniques accurately process very noisy data.
- Revolutionary constant zero second derivatives base-line fitting routine finds the best baseline. PeakFit also includes a non-parametric model for extremely complex backgrounds.
- 82 built-in nonlinear equations (18 for spectroscopy and 8 for chromatography) and up to 15 user-defined functions fit virtually all data.
- Fit up to 100 peaks at a time.
- 32-bit power and new Windows 95 interface plus, PeakFit is fully capable on Windows 3.1 and NT. With PeakFit, your accuracy will increase, and you'll find and fit your peaks faster than ever. Don't guess or rely on the accuracy of non-dedicated software made by hardware manufacturers. PeakFit far surpasses any other peak analysis package made!
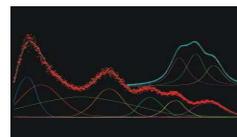
Peakfit 4.12 Features

Data input
- ASCII
- Excel
- Lotus 123
- Quattro Pro Windows
- SigmaPlot
- AIA chromatography
- dBase III+, IV
- DIF
- ASCII and spreadsheet-like editors
- Averaging digital filter

Data preparation
- Gaussian deconvolution to remove spectrophotometer instrument response smearing
- Exponential deconvolution to remove chromatographic detector response smearing
- Smoothing (Savitsky Golay, FFT Filter, Loess, Gaussian convolution)
- Real-time FFT/time domain graphical editor
- Dual-graph data sectioning with graphical data point exclusion
- Non-parametric digital filter to filter or augment data
- Compare with reference
- Subtract baseline imported from file

- Data transforms
- Area normalization
- Inspect second and fourth derivatives
- Data weighting
- Peak autoplacement
- Automatic by local maxima and residuals
- Automatic by second derivatives
- Automatic by deconvolved local maxima
- Graphical placement and adjustments
- Manual parameter adjustments
- Share and lock parameters
- Constant or variable widths and or shape in a single step

Non-linear curve fitting
- Marquardt-Levenburg algorithm
- Least-squares and 3 robust (maximum likelihood) methods
- Up to 100 peaks and 1000 parameters
- Intelligent constraints to insure fit integrity
- Sparse curvature matrix for faster fitting
- Both numeric and graphical fitting options
- Zoom-in or toggle points during fitting

83 built-in nonlinear functions
- Spectroscopy (18): Gauss Amp, Gauss area, Lorentz amp, Lorentz area, Voigt amp, Voigt area, Voigt amp approx, Voigt amp G/L, Voigt area G/l, Gauss Cnstr amp. Gauss Cnstr area, Pearson VII amp, Pearson VII area, Gauss+Lor area, Gauss*Lor, Gamma Ray, Compton Edge
- Chromatography (8): HVL, NLC, Giddings, EMG, GMG, EMG+GMG, GEMG, GEMG5-parm
- Statistical (31): Log Normal Amp, Log Normal Area, Logistic Amp, Logistic area, Laplace amp, Laplace Area, extr value amp, extr value area, log normal 4 amp, log normal 4 area, eval4 amp ailed, eval4 area tailed, eval4 amp frtd, eval4 area frtd, gamma amp, gamma area, inv gamma amp, inv gamma area, Weibull amp, Weibull area, error amp, error area, hi- sq amp, chi-sq area, student tmp, student t area, beta amp, beta area, F variance amp, F variance area, Pearson IV
- General peak (12): erfc pk, pulse pk, LDR pk, asym lgstc pk, lgstc pow pk, pulse pow pk, pulse wid2 pk, intermediate pk, sym dbl sigmoid, sym dbl Gausscum, asym dbl sigmoid,

- Transition (14): sigmoid asc, sigmoid desc, Gausscum asc, Gausscum desc, Lorentzcum asc, Lorentzcum desc, lgstcdose rsp asc, lgstcdose rsp desc, lognormcum asc, lognorrncum desc, extrcalcum asc, extrcalcum desc, pulsecum asc, pulsecum desc

User defined functions
- Up to 10 parameters per function
- Up to 15 UDF's active during fit
- Estimates can contain formulas and constraints
- Extensive mathematical, statistical, and logic functions

Baseline fit and subtract
- Automatic detection of baseline points by constant second derivatives
- Real-time fitting in conjunction with data point selection, deselection
- Background functions (10): constant, linear, progressive linear, quadratic, cubic, logarithmic, exponential, power, hyperbolic and nonparametric

Graphical review
- Component and sum curve graphs
- Residuals graphs, including distribution and stabilized normal probability plots

- Confidence and prediction intervals
- Peak labels (amplitude, center, or area)

Numerical review
- Peak characterization data: center, amplitude, integrated area, analytical area, FWHM, FW10, FWBASE, asymmetry at HM, asymmetry at 10%, first and second moments, column efficiency and resolution, percentage areas, overlap areas
- Parameter statistics: parameter values, confidence limits (90,95,99%), t-values, standard errors
- Fit statistics: Analysis of Variance, F statistic, overall standard error, r 2 value
- Data statistics: residual values, predicted y-values, confidence/prediction intervals

Output and expert options
- File export with full Generated Data: Lotus 123, Excel, QuattroPro Windows, SigmaPlot and ASCII
- Graphs to clipboard or file in BMP or WMF formats
- All numeric data in graph to clipboard in spreadsheet format

System Requirements: Microsoft Windows *95,98 and NT Pentiums or clone and above; 32MB RAM