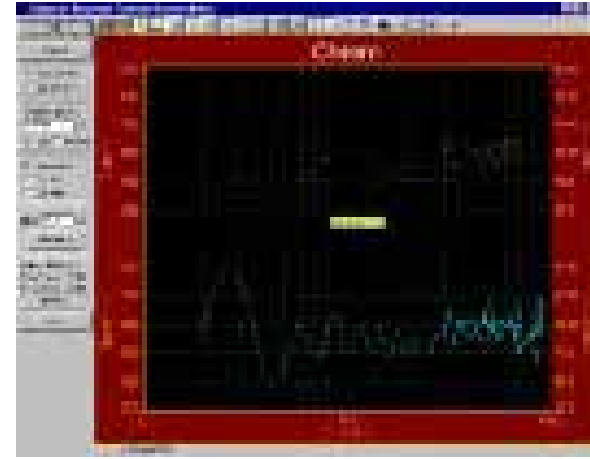


PeakLab v2

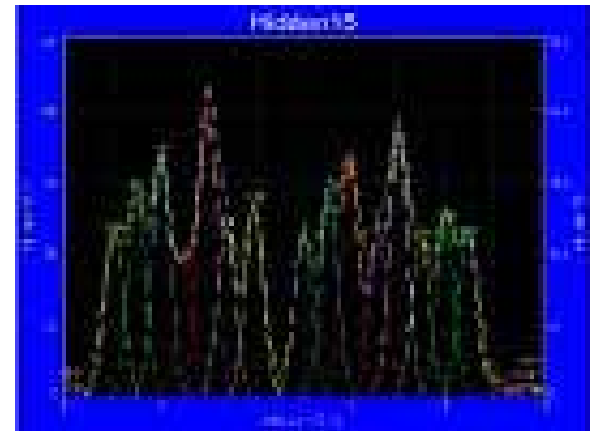
PeakLab is the automatic choice for spectroscopy, chromatography or electrophoresis

FOR SPECTROSCOPY



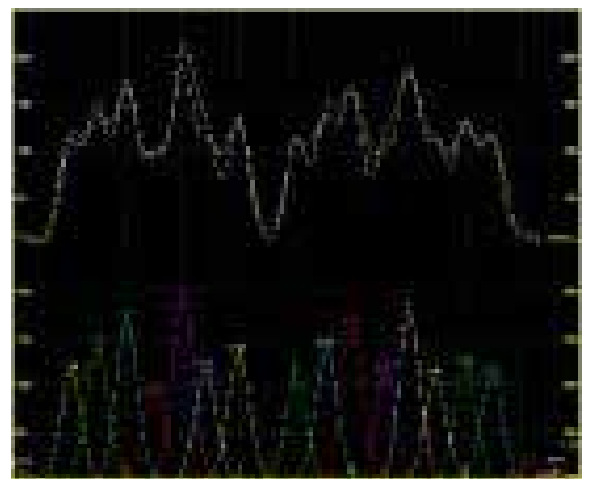
PeakLab lets you accurately detect, separate and quantify hidden peaks that standard instrumentation misses. PeakLab includes 18 different nonlinear spectral application line shapes, including the Gaussian, the Lorentzian and the Voigt — even a Gaussian plus Compton Edge model for fitting Gamma Ray peaks.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

FOR ELECTROPHORESIS



PeakLab 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 PeakLab-generated report, or they can be shown graphically. PeakLab with a hand scanner can often replace \$10,000 electrophoresis instruments — with better results!

FOR CHROMATOGRAPHY



PeakLab includes 8 different built-in equations for asymmetric peaks typically found in chromatography data:

- Exponentially-Modified Gaussian
- Haarhoff-Van der Linde
- NLC
- Giddings
- Half-Gaussian Modified Gaussian

The peak area is computed directly as a parameter within each of these functions, ensuring accuracy and enabling computation of confidence limits.

PeakLab reports:

- Column efficiency
- Resolution
- First moment (center of mass)
- Second moment
- Center (mode)
- Peak width at base and half maximum
- Asymmetry at base and 10% of maximum

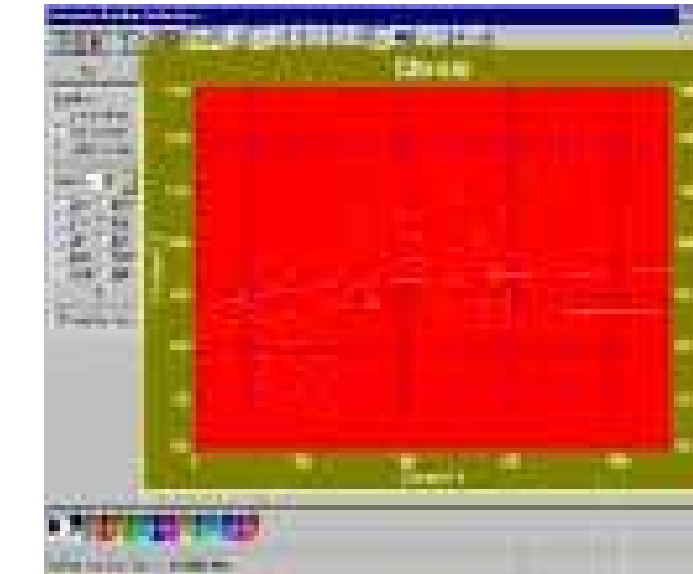
PeakLab can even deconvolve your chromatographic detector response, so you can analyze your data without instrument-induced asymmetry.

FOR SIGNAL COMPONENT ANALYSIS

Even though PeakLab is widely used by chemists, biologists, etc., many electrical engineers have found PeakLab's statistical nonlinear fitting techniques extremely useful for separating overlapping signals.

“PeakLab has been a big time saver. I wish I had found this product years ago.”

- John Spradling, Communications Engineer



Automated Peak Separation and Analysis

PeakLab's state-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 incorrect results. PeakLab helps you separate overlapping peaks by statistically fitting numerous peak functions to one data set, helping reveal obscure patterns in your data.

The background can be fit as a separate:

- Polynomial
- Exponential
- Logarithmic
- Hyperbolic
- Power model

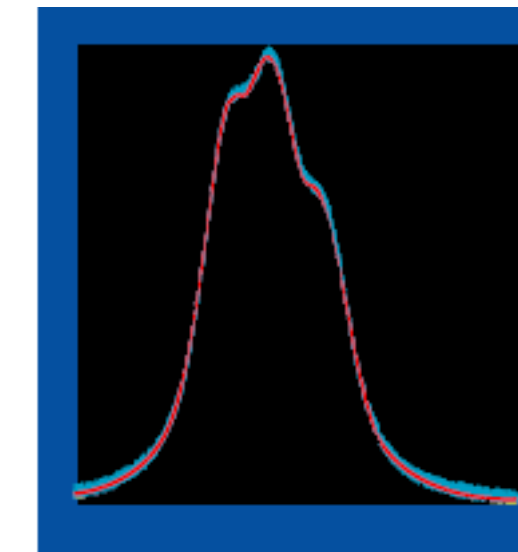
This fitted baseline is then subtracted before peak characterization data such as areas are calculated, resulting in more accurate results. Nonlinear curve fitting is essential for accurate peak analysis and conclusive research.

PEAKLAB OFFERS SOPHISTICATED DATA MANIPULATION

With PeakLab'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, PeakLab even has a digital data enhancer, which helps analyze sparse data. Only PeakLab offers so many different methods of data manipulation.

HIGHLY ADVANCED BASELINE SUBTRACTION

In this example, PeakLab'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.



FULL GRAPHICAL PLACEMENT OF PEAKS

If PeakLab'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. PeakLab'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 was created using PeakLab's builtin 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, PeakLab 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 novices can learn how to use PeakLab in no time. And if you have extremely complex or noisy data sets, the sophistication and depth of PeakLab's data manipulation techniques is unequalled.

Automated Peak Separation and Analysis

A TRUE VOIGT FUNCTION...

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. PeakLab actually uses a closed-form solution to precisely calculate the function analytically. PeakLab 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. PeakLab's precise calculation of the Voigt function is crucial to the accuracy of your analysis.



PeakLab's automation makes it as easy as 1-2-3

PEAKLAB AUTOMATICALLY PLACES PEAKS IN THREE WAYS

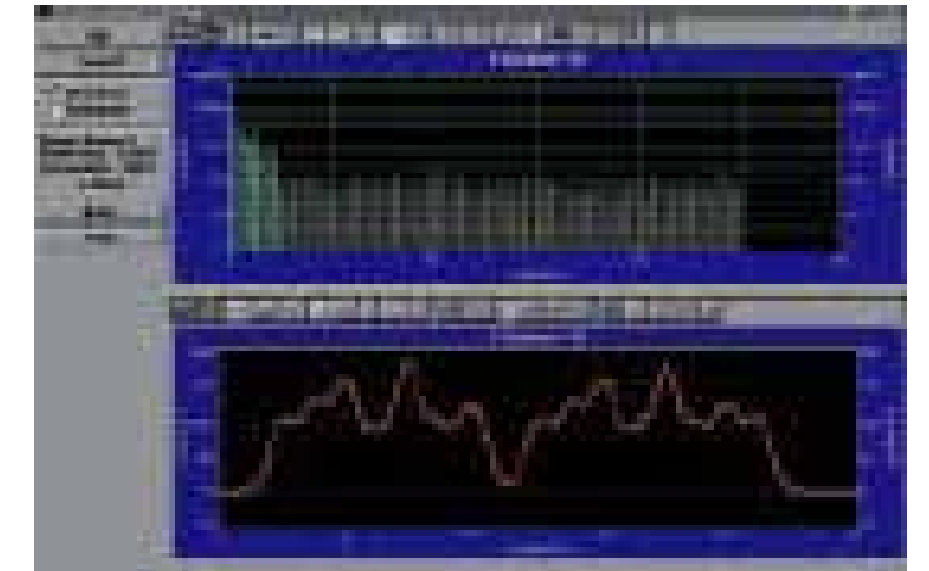
PeakLab uses three procedures to automatically place hidden peaks; while each is a strong solution, one method may work better with some data sets than the others.

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.

NONLINEAR PEAK SEPARATION AND ANALYSIS FOR SPECTROSCOPE, CHROMATOGRAPHY AND ELECTROPHORESIS

PeakLab 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! PeakLab has three different procedures to accurately characterize normal and hidden peaks.
- Graphically fit peaks yourself when you want to override PeakLab'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. PeakLab 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, PeakLab is fully capable on Windows 3.1 and NT. With PeakLab, 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. PeakLab far surpasses any other peak analysis package made!



"We know of no other comparable program that offers such sophisticated data analysis..."

Journal of the American Chemical Society Vol. 114, No. 20

Automated Peak Separation and Analysis

PeakLab Version 2 Features

Advanced Peak Separation and Analysis for Chromatography, Spectroscopy, and Chemometric Modeling

Data Input

- ASCII / AIA (net-CDF) data files
- Excel or ASCII CSV files
- Clipboard import
- Drag-and-drop from Windows Explorer
- Agilent Chemstation .ch from .d folders
- OpenLab v1: DAD, FID, FLD, VWD from .d folders
- OpenLab v1: average spectrum from .sd files
- OpenLab v2 .dx files
- Digital filter import (every nth point)
- DAD/PDA 3D chromatographic matrices
- Mass spectrometry 3D data (IRD, OpenMS)
- Spectroscopic modeling matrix import

Baseline Fit and Subtract

Baseline Identification Algorithms

- Initial/Final Linear: simplest end-point line
- Progressive Linear: ascending/descending auto-fit
- 2nd Deriv Zero: zero-second-derivative baseline detection
- SD Variation: moving-window standard deviation detection
- Whittaker pybaselines: arpls, lsrpls, brpls, drpls, aspls, iarpls, psalsa, derpsalsa, asls, iasls, airpls
- BEADS: baseline estimation and denoising with sparsity
- XPS baselines: Shirley, Tougaard

Baseline Models

- Constant, Linear, Quadratic, Cubic
- Logarithmic, Exponential, Power, Hyperbolic
- Constrained Cubic Spline
- Non-Parametric Linear (Loess-type)
- Genetic algorithm optimization of Whittaker/BEADS to mimic human baseline
- Zero baseline points (erase unwanted peaks)
- Copy baseline state across multiple data sets

User-Defined Functions (UDFs)

- Up to 60 UDFs active simultaneously
- Up to 10 parameters per UDF
- Save/load individual UDFs or full UDF libraries
- Each UDF auto-generated with <e>, <ge>, <e2> IRF convolutions
- Maple and Mathematica syntax import
- Derivative (DX, DX2) and integration (INTQUAD, INTADAPT, INTROMB) functions
- Formulas for starting estimates and constraints
- PkFnParm() and PkProp() for automatic starting estimate borrowing
- Graphical adjustment of starting estimates
- Partial derivative inspection for model validation
- Up to 8192-character function expressions
- Compiled internally for near built-in speed

Data Preparation

- Gaussian deconvolution: spectrophotometer response smearing
- Exponential deconvolution: chromatographic detector response
- IRF (Instrument Response Function) deconvolution
- Voigt spectroscopic deconvolution
- Section data: isolate X ranges of interest
- Smoothing: FFT Filtering, Loess, Gaussian Convolution, Savitzky-Golay
- AI Expert auto-smoothing level optimization
- Savitzky-Golay 1st-4th derivative generation
- Interpolate / Upsample for uniform X-spacing
- Fourier domain (FFT) graphical filtering
- Data transforms (log, arithmetic, normalization)
- Data weighting options
- View and compare multiple data sets
- Append PeakLab data files
- Digital filter utility: consolidate up to 256 ASCII/AIA files

Peak Autoplacement

- Fit Local Maxima Peaks: auto-places all resolved peaks
- Fit Hidden Peaks – Residuals: finds hidden peaks from residual maxima
- Fit Hidden Peaks – Second Derivative: finds hidden peaks from Savitzky-Golay D2 minima
- Graphical placement: left-click anchor for center, amplitude, width, shape
- Numeric adjustment popup: change model, lock/share parameters per peak
- Common parameters dialog: simultaneous multi-peak adjustment
- Massively Parallel Peak Fitting (MPPF): automated batch model search
- Genetic algorithm (DE) pre-fit for global optimization
- Import scan parameter estimates from file
- Segment fit for large multi-peak data sets
- Automatic model experiment and optimum-model search

Numerical Review

- Fitted parameters: r^2 , DF-adj r^2 , Fit Std Err, F-value, ppm unaccounted variance
- Equivalent parameters: GenHVL \leftrightarrow GenNLC conversion
- Measured values: amplitude, center (mode), FWHM, FW Base, Asym50, Asym10
- Integrated area, % area, mean, SD, skewness, kurtosis
- Analytic moments: closed-form area, mean, SD, skewness, kurtosis
- Deconvolved moments for IRF, ZDD, and concentration-distortion layers
- Advanced area analysis: apex asymmetry, non-overlap areas, cumulative quantiles
- Parameter statistics: value, std error, t-value, confidence limits (90/95/99%)

Nonlinear Curve Fitting

- Levenberg-Marquardt algorithm (primary)
- Least-squares and robust (maximum likelihood) fitting
- Sparse curvature matrix for faster fitting
- Genetic algorithm (DE) global pre-fit
- Parallel processing support
- Intelligent parameter constraints to ensure fit integrity
- Lock individual parameters (held constant during fit)
- Share parameters across peaks (common value)
- Variable or constant widths and shapes in a single step
- Convergence tolerance user-adjustable (default 1E-6)
- IRF (Instrument Response Function) convolution fitting
- ZDD (Zero-Distortion Density) higher-moment models
- Baseline-with-peaks simultaneous fitting (Hidden Peaks options)
- Fit up to 25 data sets simultaneously
- Numeric and graphical fitting options

Graphical Review

- Component and sum curve graphs Y + Y2 dual-axis
- IRF Deconv., Partial Deconv., Full Deconv. peak renderings
- State-1 / State-2 rendering for two-component ZDD models
- Confidence and prediction interval overlays (90/95/99%)
- Residuals graph with distribution and SNP (normal probability) plots
- Explore: graphical matrix of parameter vs. property relationships
- Map experimental process variables to data sets
- Peak labels: amplitude, center, area, moments, and more
- Selective review: compare any subset of fitted data sets
- Average multiple fits with CV% analysis
- Array layout control for multi-data-set display
- Publication-quality graph copy, save (BMP, WMF, PNG), and print
- Chromatography analysis: Nmoment, Ndeconv, Nmodel, Ngauss theoretical plates
- Retention (capacity factor k), resolution Res(HW) and Res(Stat)
- Nonlinear regime fraction (fracNL)
- Overlap areas matrix, ANOVA, Analysis of Variance
- Average multiple fits with full CV% summary

Built-In Nonlinear Peak Functions

Chromatography Models

- HVL (Haarhoff-Van der Linde, full range)
- NLC (Non-Linear Chromatography, full range)
- GenHVL, GenNLC (generalized families)
- Gen2HVL, Gen2NLC (twice-generalized)
- GenHVL/GenNLC with ZDDs: [Z], [Y], [T], [V], [G], [E], [Q], [S], [K], [Yp], [YpE], [Yp2], [Yp2E], [W]
- EMC, GMG, GEAMG, E2AMG, E2xMG, RHVL
- Giddings, Gaussian (chromatographic)
- LN4 Generalized Normal
- IRF specializations: <e>, <ge>, <e2>, and more

Spectroscopy Models

- Gaussian (amplitude and area)
- Lorentzian (amplitude and area)
- Voigt (4 variants: amplitude, area, component widths)
- Generalized Voigt
- Pearson VII (amplitude and area)
- Constrained Gaussian
- Gamma Ray / Compton Edge
- Convolutions: Gaussian and Kinetic Decay

Statistical & Other Models

- Asymmetric Generalized Normal (multiple variants)
- LN4 Generalized Normal
- Transition functions (sigmoid, Gaussian desc., Lorentz desc., etc.)
- Miscellaneous peak functions
- User-defined peaks with <e>, <ge>, <e2> IRF auto-generated

Output and Expert Options

- Export numeric summary to ASCII CSV (comma, tab, or space delimited)
- Export data summary with X, Y, fitted curve, and component peaks
- Export to Windows INF file for programmatic parsing
- Export to extended AIA net-CDF file
- Export fit(s) to CSV or Apache Parquet file
- Export fit(s) directly to DuckDB database
- Convert PeakLab database to CSV or Parquet
- Numeric Summary database export for longitudinal tracking
- Graph copy to clipboard (BMP / WMF)
- Graph save to file
- MS Word stream output of graphs
- Evaluate fit model: function, derivative, cumulative tables at any X
- Map peak identifications/labels for reporting