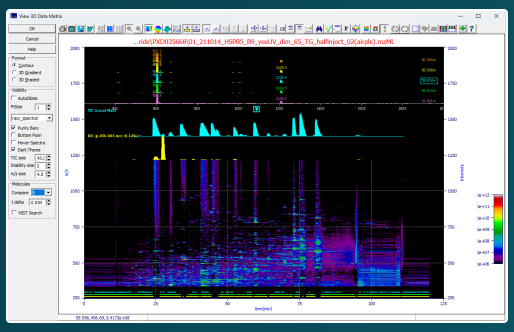
R²N SOFTWARE · PEAKLAB

PeakLab

version 2.0

Peak fitting, deconvolution and spectral modelling



Your baseline is not a separate problem.

PeakLab fits the baseline and the peaks as one model, resolves components that overlap too closely to integrate, and reads the formats your instruments actually write. Built on thirty years of peak-fitting heritage, and the successor to PeakFit.

PeakLab v2.0

The next-generation peak fitting software for spectroscopy and chromatography: generalized chromatographic models, instrument response deconvolution, integrated baselines and native mass spectrometry workflows.

ADVANCED MODELLING, NOT BASIC CURVE FITTING

Mathematically defensible results from real instrument data

Generic fitting tools work best on clean, well-separated data. Real chromatograms and spectra are neither. Peaks overlap, baselines drift, instruments impose their own response on every measurement, and the interesting component is often the one hiding inside a shoulder. PeakLab is built for that case: it treats the baseline as part of the model rather than something you subtract first, it resolves co-eluting and hidden components instead of integrating around them, and it produces parameters tied to real system behaviour rather than coefficients with no physical meaning.

What that changes in practice

- **Baseline is part of the model.** Fitted simultaneously with the peaks, so the two cannot trade error between them.
- **Built for overlapping peaks.** Co-elution, shoulders and hidden components are the design case, not an edge case.
- **Designed for real instrument data.** Native Agilent, OpenLab, AIA/netCDF and mzML import — not CSV only.
- **Scientifically defensible results.** Full statistical reporting, confidence and prediction intervals, and reproducible models you can put in a paper or a submission.

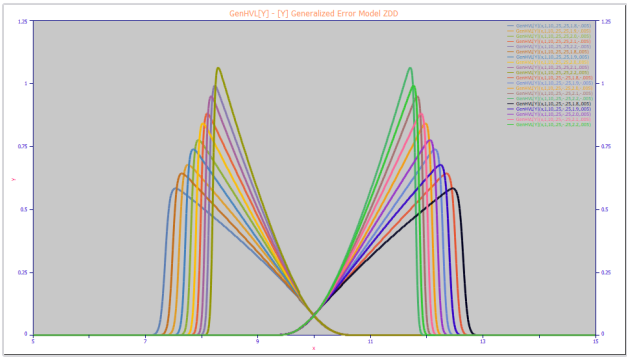
> *"Unlike generic tools, PeakLab provides mathematically defensible and reproducible results built for real instruments."*
>
> **R²N Software**

PEAK MODELS

Models that describe the chemistry, not just the shape

PeakLab's chromatographic models are derived from the underlying transport and partitioning behaviour rather than fitted as arbitrary asymmetric shapes. The generalized HVL and NLC families — **GenHVL**, **Gen2HVL** and **GenNLC** — each carry a full set of variants that account for a different distortion: generalized error, Giddings, Kubelka, Student's t, Voigt, Weibull and more, each selectable as a bracketed form such as GenHVL[Y] or Gen2HVL[V].

Alongside them sit the classical and statistical shapes you would expect — Gaussian, Lorentzian, Voigt and generalized Voigt, generalized normal and LN4, Pearson VII, Giddings, EMG, GMG, E2AMG, G2AMG and GEAMG — plus transition functions, constrained Gaussians, XPS spectral shapes, Compton edge and gamma-ray forms, and your own user-defined peaks.



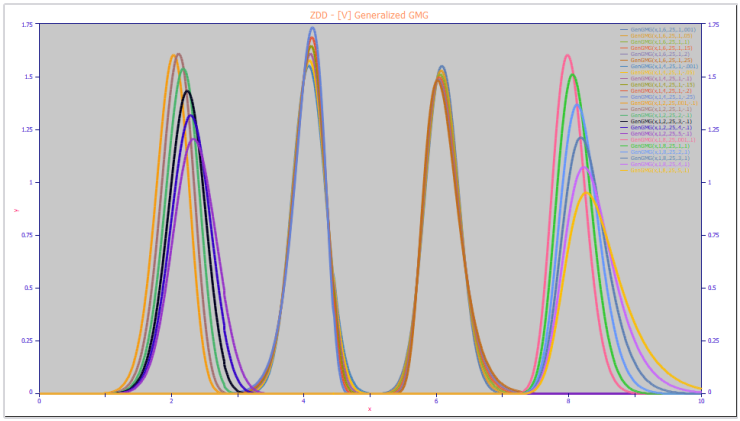
The GenHVL[Y] generalized error family across its parameter range — fronted on the left, tailed on the right, from a single model rather than two different equations.

Instrument response, removed properly

Every detector imposes its own response function on the measurement. PeakLab determines the instrument response function from your own data — from standards, from a fronted or tailed peak, or from a GC reference — and then deconvolves it, so the parameters you report describe the chemistry rather than the chromatograph. The IRF can be estimated, fitted, saved and reapplied across a method.

Zero distortion deconvolution

ZDD removes the instrument's contribution without introducing the ringing and negative lobes that ordinary Fourier deconvolution produces. It is available across the same generalized model variants as the peak families, so the deconvolved result stays consistent with the model you fitted. Deconvolution levels and deconvolved moments are reported directly.



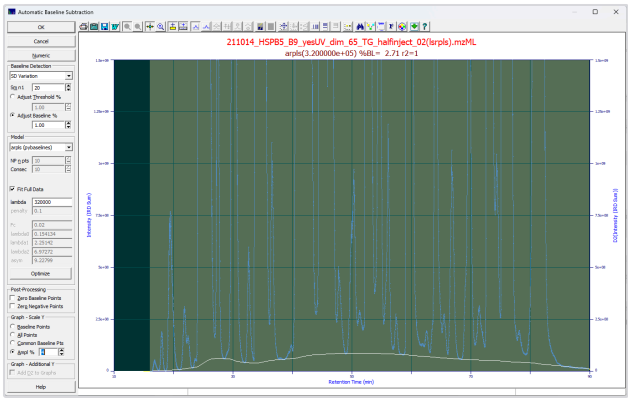
ZDD across the Voigt variant's parameter range. Deconvolution is a property of the model, not a post-processing filter applied afterwards.

BASELINES

Fitted with the peaks, not subtracted before them

Subtracting a baseline before fitting bakes an assumption into the data and hides the error it introduces. PeakLab fits the baseline as part of the model, so peak area and baseline curvature cannot quietly absorb one another.

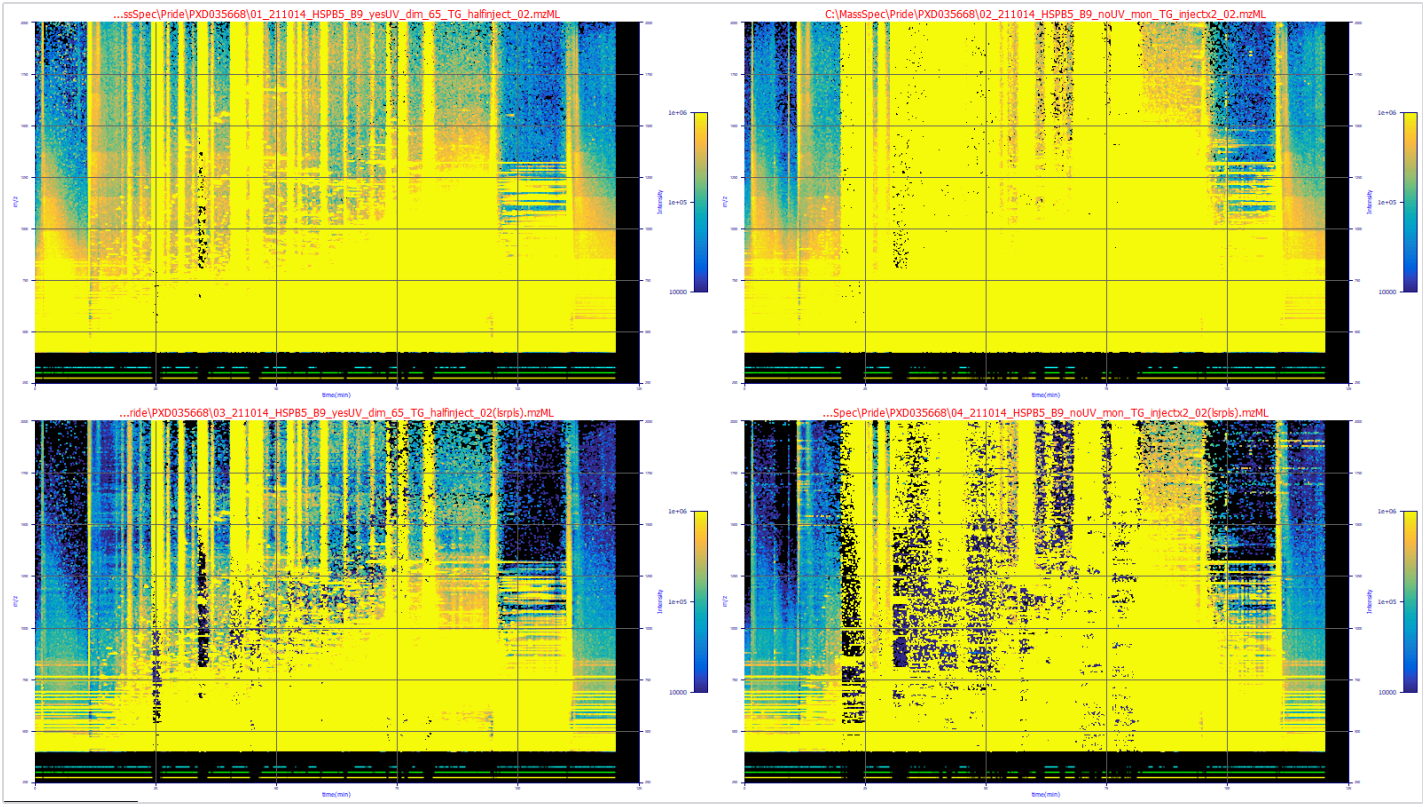
The baseline library covers the methods each discipline actually uses: **Bohlmann-Whittaker** and the wider Whittaker family for smooth drift, **BEADS** for simultaneous baseline estimation and denoising, and **Shirley** and **Tougaard** for XPS, where the background is physics rather than drift. Baseline optimisation runs as part of the fit, and DAD/PDA data has its own baseline filter.



Baseline selection and optimisation, applied live against the data with the fitted peaks in view.

MASS SPECTROMETRY

Native LC-MS workflows, not a converted spreadsheet



Background filtering across a full LC-MS matrix. Noise is removed from the m/z dimension before peaks are fitted in the time dimension.

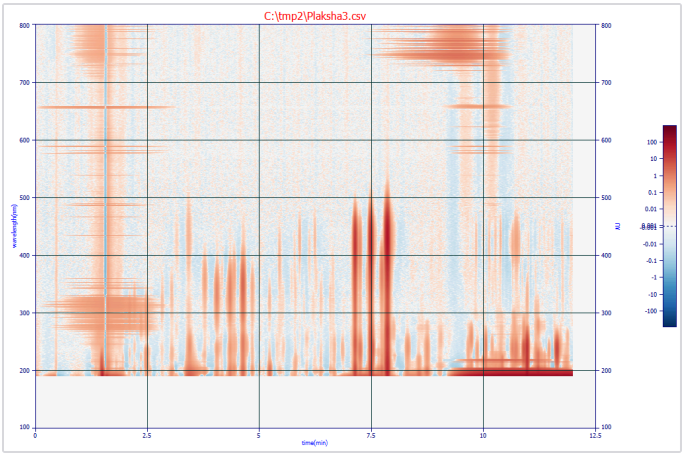
PeakLab reads **mzML** directly and works with the data as a time-versus-m/z matrix rather than as a flattened trace. Total ion and extracted ion chromatograms are generated from the matrix, background is filtered in the mass dimension, isotope clusters and overlapping ions are resolved by fitting rather than by integration thresholds, and purity bars show where a chromatographic peak is spectrally homogeneous and where it is not. A NIST search is available against the resolved spectra, and the OpenMS and IRD workflows are supported for pipeline use.

THREE-DIMENSIONAL DATA

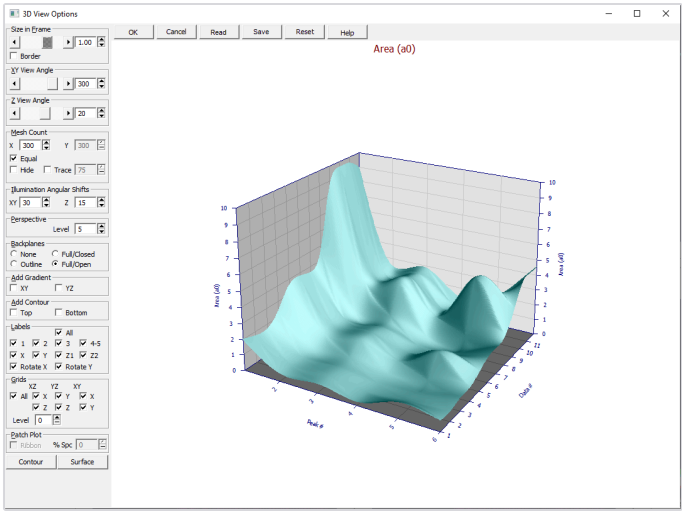
DAD, PDA and spectral surfaces

Diode-array and photodiode-array detectors produce a surface, not a trace. PeakLab views that surface directly — as a contour map, a 3D gradient or a shaded rendering — reduces the matrix to the region that matters, and lets you select individual spectra at any retention time for modelling.

MCR-ALS — multivariate curve resolution by alternating least squares — recovers the pure component spectra and their concentration profiles from the mixture, which is the right tool when components co-elute so closely that no chromatographic model will separate them.



A PDA matrix on a symmetric-log absorbance scale, wavelength against time. The diverging scale makes both weak positive and negative excursions visible at once.



Fitted results as a surface across a sequence of data sets — how a parameter moves with an experimental variable. View angles, mesh count, illumination and backplanes are set live.

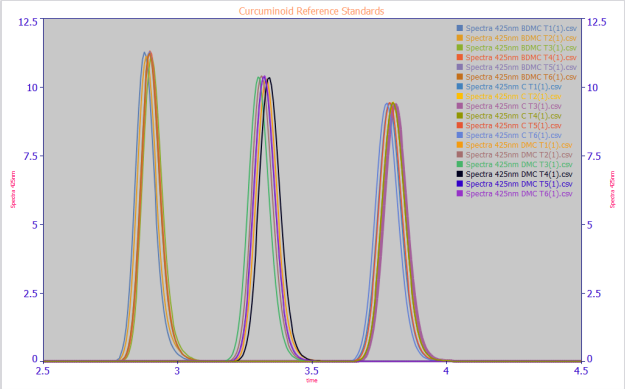
SPECTRAL AND MULTIVARIATE MODELLING

From resolved peaks to a predictive model

Resolving a spectrum is often only the first half of the job. PeakLab's **GLM** modelling takes the fitted peak parameters — areas, widths, centres, asymmetries — and builds a predictive model from them, with full-permutation model search, significance testing, performance analysis and prediction against new data.

Because the predictors are physically meaningful peak parameters rather than raw absorbances, the resulting models tend to be smaller, more interpretable and more stable than PLS or PCR built on the full spectrum. PeakLab documents that comparison directly.

Worked workflows are included for FTNIR, NIR field-site data and UV-Vis modelling.



UV-Vis spectral modelling: component bands fitted beneath the measured spectrum, ready to serve as predictors in a GLM model.

THE FITTING ENGINE

Up to 1,000 peaks, fitted in parallel

Massively parallel peak fitting

MPPF distributes the optimisation across every available core, so data sets that would once have been left to run overnight finish while you watch. Parallel processing applies to the model search as well as to the fit itself.

Finding the peaks you cannot see

Hidden components are detected from the residuals or from the second derivative, and local maxima can be fitted directly. Model discovery and the optimum-model search run the candidate families against your data and rank what fits, rather than asking you to nominate a shape in advance.

Optimisation that copes with real data

Robust fitting limits the influence of outliers. A genetic algorithm handles the cases where gradient methods stall in a local minimum. Graphical fitting lets you place and adjust components by hand when you already know what should be there, and segment fitting confines the work to a region of interest.

Signal conditioning

Fourier-domain filtering with selectable tapering windows, Fourier estimation of spectra and signal-to-noise, interpolation and upsampling, smoothing, sectioning, transforms and weighting — all available before the fit and all reversible.

SUPPORTED APPLICATIONS

Where PeakLab is used

Mass spectrometry

MS and LC-MS. Resolve isotope clusters and overlapping ions, filter background in the mass dimension, and generate TIC and XIC traces from the full matrix.

Chromatography

HPLC, GC, SFC, IC and SEC. Accurate peak integration despite drift and overlap, with instrument response removed and the baseline fitted alongside the peaks.

Spectroscopy

UV-Vis, IR, FTNIR, Raman, NMR, microwave, XPS and Auger. Separate complex overlapping signals with physically correct backgrounds.

OUTPUT AND INTEGRATION

Results that leave the program cleanly

Numeric summaries, data tables, residuals and the full statistical report export to MS Word or generic RTF with the graphs embedded at full resolution. Numeric output streams to a database, and the modern analytics formats are supported directly: **CSV and text**, **Apache Parquet**, **DuckDB**, **Zarr and TileDB**, and **SQL via Arrow or ODBC**. Models can be exported for Maple and Mathematica, and saved fits can be managed, reimported and reapplied to new data.

A Python 3.12 runtime ships with the program, so analyses can be scripted and PeakLab can sit inside an automated pipeline rather than at the end of one.

SPECIFICATIONS

PeakLab 2.0 Features

- New in PeakLab 2.0

INTERFACE

- Native 64-bit application for Windows 10 and 11
- Main data window with spreadsheet-style editor and live graphing
- Customisable toolbar; peak popup for direct component editing
- Graphical fitting — place and adjust components by hand
- Explore mode for rapid inspection across data sets
- Manage saved fits; reapply a model across a method
- Advanced online help with worked tutorials
- Dark theme for the 3D data matrix viewer new

DATA INPUT

- Native mzML mass spectrometry import new
- OpenMS and IRD mass spectrometry workflows new
- Agilent and OpenLab native data import
- AIA/netCDF chromatography interchange
- ASCII and text import with a built-in editor
- Import data sets from an existing model
- Import scan parameter estimates
- Import spectroscopic modelling sets
- DAD/PDA three-dimensional matrices

DATA PREPARATION

- Fourier-domain filtering with selectable data tapering windows
- Fourier estimation of spectra; Fourier signal-to-noise estimation
- Smoothing, interpolation and upsampling
- Sectioning, transforms and weighting
- First derivative spectra
- Combine or partition data matrices
- Background filtering of MS data in the mass dimension new
- DAD/PDA baseline filtering and matrix reduction new

CHROMATOGRAPHIC PEAK MODELS

- GenHVL generalized chromatographic family with 14 distortion variants: [E] [G] [K] [Q] [S] [T] [V] [W] [Y] [Yp] [Yp2] [YpE] [Yp2E] [Z] new
- Gen2HVL second-generation family with its own specialisations new
- GenNLC generalized NLC family with [T] [V] [Y] [Z] variants new
- HVL and NLC full-range models
- RHVL; Giddings
- Generalized two-state HVL models
- Gradient HPLC peak models
- Common distortion model
- Preparative and overloaded peak fitting

SPECTROSCOPIC AND STATISTICAL PEAK MODELS

- Gaussian; constrained Gaussian; Lorentzian
- Voigt and generalized Voigt
- Generalized normal; LN4 generalized normal
- Pearson VII
- EMG, GMG, E2AMG, E2xMG, G2AMG, GEAMG
- Transition functions
- XPS spectral shapes
- Compton edge; gamma-ray forms
- Miscellaneous peak functions
- User-defined peaks with full expression parser
- Statistical functions library

INSTRUMENT RESPONSE AND DECONVOLUTION

- IRF determination from your own data new
- IRF estimation from standards, from GC data, and from fronted or tailed peaks
- IRF model fits, saved and reapplied across a method
- ZDD zero distortion deconvolution across all model variants new
- Gaussian and Kubelka convolutions
- Voigt deconvolution
- Selectable deconvolution levels
- Deconvolved moments reported directly

BASELINE MODELLING

- Baseline fitted simultaneously with the peaks

- Bohlmann-Whittaker and the wider Whittaker family
- BEADS — simultaneous baseline estimation and denoising new
- Shirley and Tougaard XPS backgrounds
- Baseline optimisation as part of the fit
- Dedicated DAD/PDA baseline filter

FITTING AND OPTIMISATION

- Up to 1,000 peaks fitted simultaneously new
- MPPF — massively parallel peak fitting across all available cores new
- Nonlinear least-squares fitting with high-precision kernels
- Robust fitting for outlier resistance
- Genetic algorithm for difficult optimisation surfaces
- Automatic peak detection
- Hidden peak detection from residuals and from the second derivative
- Fit local maxima peaks
- Model discovery and search for optimum model
- Segment fitting over a region of interest
- Graphical fitting with manual component placement
- Fit strategy control and peak fit preferences
- Monte Carlo evaluation

MASS SPECTROMETRY

- mzML native import new
- Time-versus-m/z data matrix view with contour, 3D gradient and shaded formats new
- TIC and XIC generation from the full matrix new
- Spectral purity bars across a chromatographic peak new
- NIST library search against resolved spectra new
- Isotope cluster and overlapping ion resolution by fitting
- Background filtering in the mass dimension

MULTIVARIATE AND SPECTRAL MODELLING

- MCR-ALS multivariate curve resolution by alternating least squares new
- GLM modelling from fitted peak parameters new
- Full-permutation GLM model search
- GLM significance, performance analysis and prediction
- Generate and modify the GLM data matrix
- Documented comparison against PLS, PCR and direct methods
- Worked FTNIR, NIR field-site and UV-Vis modelling workflows
- Map experimental process variables to peaks
- Map identification to peaks

THREE-DIMENSIONAL DATA

- DAD/PDA 3D chromatography and spectroscopy
- View and reduce the 3D matrix; select individual PDA spectra
- Contour, 3D gradient and shaded surface rendering
- Adjustable mesh count, illumination angles, perspective and backplanes
- Contours added to the top or bottom of a surface
- Full 3D animation through an angle sequence
- Surface and contour property control, applied live

ANALYSIS AND OUTPUT

Numerical

- Full numeric summary with fitted parameters and standard errors
- Confidence and prediction intervals
- Data summary and data table statistics
- Deconvolved moments; peak areas, centres, widths and asymmetries
- Evaluation procedure with automated table generation
- Numeric summary database export

Graphical

- Fitted peak graph with component overlay and peak labels
- Residuals graph
- Reference lines
- Graph colours, scaling, point format, custom titles — 2D and 3D
- View Function(X); view and compare data sets
- Graph all data sets in a spectral series
- Print preview for graphs and text

EXPORT AND INTEGRATION

- MS Word and generic RTF report streaming with embedded graphs
- CSV and text
- Apache Parquet new
- DuckDB new
- Zarr and TileDB new
- SQL via Arrow or ODBC new
- Maple and Mathematica model export
- Graph export as bitmap, metafile and enhanced metafile
- Embedded Python 3.12 runtime for scripted analysis new

SYSTEM REQUIREMENTS

- Windows 10 or Windows 11, 64-bit new
- x64 processor; multi-core recommended for MPPF new
- 8 GB RAM minimum; 16 GB or more recommended for LC-MS and DAD/PDA matrices
- 1 GB of available disk space
- 1920 × 1080 display or higher recommended
- Internet connection required for licence activation