Software Solutions for IR, NMR, NIR, MS, UV-Vis, & Chromatography

KnowItAll® Analytical Edition
Whether you use one or more techniques, KnowItAll® Spectroscopy Software has the right solution for your lab!

Bio-Rad’s KnowItAll Informatics System, Analytical Edition offers solutions to identify, analyze, and manage spectral data. It supports multiple instrument vendor file formats and techniques, including IR, Raman, NIR, NMR, MS, UV-Vis, & chromatography. So whether you use one or more techniques, it’s the ideal vendor-neutral solution for your lab.

KnowItAll eliminates the need for multiple software packages with powerful tools integrated into a single, easy-to-use interface. We continually add spectral intelligence to our software, which also includes patented tools not available in other packages.

Combined with the world’s largest spectral reference database—including Bio-Rad’s renowned Sadtler™ libraries and spectra from trusted partners—KnowItAll Software gives chemists the most advanced technology available for fast, accurate spectral analysis!

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Powerful tools integrated into a single, easy-to-use interface.

Move seamlessly between tasks: spectral identification, search, processing, database building, prediction, mixture analysis, structure drawing, reporting, and more.

Handle multiple vendor file formats and techniques—making it the ideal vendor-neutral solution for your current and future laboratory needs.
What Is Included?

KnowItAll integrates multiple types of analytical data (IR, Raman, NIR, MS, UV-Vis, chromatograms, structures) and tools into a single interface, so chemists can perform multiple tasks in relation to that data—and ultimately extract greater knowledge from it. Easily transfer information from one tool to another and move from one task to the next, without having to leave the main interface or open another program.

Data Toolbox

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<td>One-click spectral identification tool: to perform applicable basic analyses (single and multi-component search, peak search, and functional group analysis) on an unknown spectrum</td>
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<td>SearchIt™</td>
<td>Advanced database searching including simultaneous multi-technique search</td>
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<td>Mixture Analysis</td>
<td>Advanced analysis of experimental spectral data of mixtures</td>
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<td>MineIt™</td>
<td>Multi-technique spectral database building / management and data mining—includes patented Overlap Density Heatmap technology to visualize similarities and dissimilarities in datasets.</td>
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<td>Deformulation Expert™</td>
<td>Reverse engineering of IR spectra of commercial products into pure components</td>
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<td>QC Expert™</td>
<td>Perform a QC comparison of a sample IR or Raman spectrum against a reference spectrum</td>
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<td>AssignIt™ NMR</td>
<td>Add assignments to NMR databases</td>
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Optimized Corrections Technology

**New Patent-Pending Technology to Find Optimal Spectral Matches**

Searching is not always a straight-forward process. What if there are problems with your query spectrum, library reference spectra, or both? If there is, you may never find the right match—even if it is in the library. Bio-Rad offers a unique patent-pending solution to solve this complex problem and lead you to the best results. Bio-Rad's Optimized Corrections is a spectrally intelligent solution built into KnowItAll's ID Expert, SearchIt, Mixture Analysis, and Deformulation Expert. It performs a computationally complex set of corrections on all query and reference spectra in a search to find the optimal match between the query and each reference spectrum. Multiple corrections are applied automatically to compensate for differences between spectra caused by the variability of different instruments and accessories as well as other factors, including human error. Corrections include: baseline correction, clipping, horizontal shift, vertical shift, intensity distortion, and ATR correction. See application note at www.knowitall.com/optimizedcorrections
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See KnowItAll in action at www.knowitall.com/youtube
Spectral Identification

The Ideal First-Pass Spectral Identification Tool

When it comes to identifying unknown spectra, it’s difficult to figure out where to begin. Bio-Rad’s KnowItAll ID Expert offers both novices and experts the perfect place to start.

KnowItAll ID Expert is a completely new technology to provide the fastest, most accurate answers possible to scientists identifying unknown spectra. The spectral intelligence built into KnowItAll ID Expert when used with Bio-Rad’s high-quality KnowItAll Spectral Libraries*—the world’s largest collection—is the recommended first step for anyone identifying unknown spectra.

How Does It Work?

- The user simply opens an unknown spectrum and KnowItAll ID Expert automatically performs a series of basic analyses (single and multi-component search, peak search, and functional group analysis) and summarizes the results to give a complete overview of all possibilities for the unknown.
- If there are problems with the unknown spectrum or the reference spectra, ID Expert has the spectral intelligence to identify and fix some of these issues using Bio-Rad’s patent-pending Optimized Corrections technology.
- Once the user has identified the unknown spectrum, a PDF report can be generated with a single click.

Includes Optimized Corrections Technology

If there are problems with the unknown spectrum or the reference spectra, SearchIt has the spectral intelligence to identify and fix some of these issues using Bio-Rad’s patent-pending Optimized Corrections technology to ensure the best results possible.

*KnowItAll Spectral Libraries are a KnowItAll Option / Add-On
Advanced Database Searching

SearchIt allows users to import data and search against user-generated databases or KnowItAll Spectral Libraries. Searches are fully customizable and driven by powerful algorithms. Search by name, structure, substructure, properties, spectra, and peak—in any combination.

Multi-Technique Spectral Searching

KnowItAll is the world's first and only search system capable of searching spectra in multiple analytical techniques simultaneously from one or many databases. For example, query an NMR spectrum in one database and a mass spectrum in another database at the same time to find the most relevant hits from each database linked to one another by chemical structure.

Advanced Spectral Searching

SearchIt permits both full spectrum and peak searching. Euclidean Distance, First Derivative Euclidean Distance, Second Derivative Euclidean Distance, and Correlation algorithms are available for full-spectrum searches. For peak searches, the user can manually select peaks or use the automated peak picking capability.

Includes Optimized Corrections Technology

If there are problems with the unknown spectrum or the reference spectra, SearchIt has the spectral intelligence to identify and fix some of these issues using Bio-Rad's patent-pending Optimized Corrections technology to ensure the best results possible.
Advanced Analysis of Experimental Spectral Data of Mixtures

This tool deconvolutes components of a mixture by analyzing a spectrum. It allows comparison of a sample spectrum against KnowItAll databases of a user's own proprietary spectra as well as any licensed KnowItAll reference databases.

The result is a series of composite spectra, each accompanied by the individual component spectra that comprise the composite spectrum as well as the residual spectrum (the difference between the query spectrum of the actual mixture and the composite spectrum). The composite spectra are ranked by how closely they resemble the query spectrum.

Includes Optimized Corrections Technology

If there are problems with the unknown spectrum or the reference spectra, KnowItAll's Mixture Analysis has the spectral intelligence to identify and fix some of these issues using Bio-Rad's patent-pending Optimized Corrections technology to ensure the best results possible.

Include or Exclude Components

To better narrow down the analysis, KnowItAll offers options to include known components or conversely to exclude components.
Spectral Database Building and Management

Chemists and spectroscopists produce valuable data every day within their organizations. Because Bio-Rad Informatics Division’s primary business is creating spectral databases, the KnowItAll solutions have been built through years of experience in doing just that—building databases.

Build Multi-Technique Databases from Various Vendors

Researchers can build searchable databases that include one or more analytical techniques (IR, Raman, NMR, Near IR, MS, UV-Vis, chromatography), chemical structures, and other metadata. So even if a laboratory’s analytical instruments come from multiple manufacturers, KnowItAll can archive the data.

Key Features

Build Databases with Spectral & Chromatographic Data

- Build databases with one or more analytical techniques
- Build databases with multiple spectral scans in the same record
- Import analytical data even if laboratory has instruments from multiple vendors
- One-click import of common native instrument file formats or *.csv format (spreadsheet)
- Enhance each record with peak information, structures, and properties, such as source of sample, boiling point, etc.
- Import multiple structure formats (with stereochemical bonds and identifiers)
- Use “Batch Import and Export” for efficient handling of spectra, structures, and property files
- Supports unrestricted spectral range and resolution - Store spectra at the precise range and resolution at which each spectrum was measured rather than being forced to conform to a fixed range and resolution
- “Auto-Property” computes values such as formula, molecular weight, etc. for entire datasets
- Make database more powerful by attaching spreadsheets, MSDS, and other documents or adding hyperlinks to web pages
- Create cross-reference from record to data from another technique; i.e., an NMR spectrum can be linked to an IR spectrum
- Quickly add properties and structures from PubChem to your database

Customize Databases

- Databases can be customized to meet laboratory specifications
- Users can create custom fields to support associated metadata relevant to their work
- Choose from three types of property fields: text, numeric, hyperlink
- Generate “preferred property” forms so users enter properties consistently
- Set spectral parameters such as x- and y-resolution

Extract the Most Information from Your Data

- Fully integrated with other KnowItAll applications for processing, database searching/mining, structure drawing, processing, reporting, and more
Multi-Technique Viewing & Mining

With Minelt, users can view reference databases, user-created databases, or search results. Access databases containing many types of data, such as IR, Raman, NMR, NIR, MS, UV-Vis, chromatograms, structures, physical properties, and more. Since analytical databases can contain one or more techniques in the same record, this tool is ideal for accessing databases of reference spectra.

Advanced Datamining Capabilities

Compare any two variables from a database using a scatter plot diagram to separate data that follow a desired trend from that which does not. Select any point on the scatter plot to display the compounds associated with that record.

Patented Overlap Density Heatmaps Technology for Data Mining & Analysis

Traditionally, the visualization of multiple spectra takes place in an overlay, offset, or stacked plot. These traditional plotting methods, however, obscure trends when viewing large amounts of data. With Overlap Density Heatmaps, users can visualize trends and assess similarities and dissimilarities in massive amounts of data. Specifically, this technology allows the user to see common features of overlapped objects (such as spectra) by color coding spectral areas from highest to lowest overlap.

For example: This plotting feature is useful in the analysis of spectral searches for samples run in multiple techniques by plotting the quality of database search results (Hit Quality Indices - HQIs) against each other (e.g., IR HQI versus Raman HQI).

Overlap Density Heatmaps: An Example

Traditional Stacked Display

Thirty-one IR spectra of alkanes are shown. While some trends appear, the extent of the trends is obscured.

OD Heatmap
OD Level = 100

An Overlap Density Heatmap showing only those areas of overlap common to all spectra.

OD Heatmap
OD Level = 0

An Overlap Density Heatmap of the thirty-one alkanes shown revealing all overlap levels. High levels of overlap are displayed in red; low levels are displayed in violet.
Reverse Engineer Commercial IR Spectra

KnowItAll Deformulation Expert assists scientists with:

- Reverse engineering of formulated products
- Competitive analysis
- Patent infringement litigation
- Verification of product raw materials

Simply open a spectrum of a formulated product and KnowItAll Deformulation Expert automatically searches for pure components that make up the formulation of the commercial product.

Includes Optimized Corrections Technology

If there are problems with the unknown spectrum or the reference spectra, Deformulation Expert has the spectral intelligence to identify and fix some of these issues using Bio-Rad’s patent-pending Optimized Corrections technology to ensure the best results possible.

*Deformulation Expert requires a subscription to the KnowItAll IR Spectral Library to view unlocked results.*
Bio-Rad’s KnowItAll QC Expert software performs a rapid quality check of a sample IR or Raman spectrum against a “gold standard” user spectrum to verify that a material meets control specifications.

**Key Features**

- Perform QC comparison of a sample spectrum to a selected reference spectrum
- Validate results by also comparing the sample to a reference database to ensure the sample not only matches the selected reference spectrum, but that it also does not match anything else in the database
- Define user privileges, reference data, and other settings to ensure technicians follow set protocols and focus on output
- Identify problems with the sample spectrum - QC Expert’s built-in spectral intelligence identifies issues and suggests ways to fix them
- Generate tamper-evident, digitally-signed reports
- 21 CFR Part 11-compliant
Create Fully Assigned NMR Databases

AssignIt NMR allows users to add NMR assignments to the structures in $^1$H, $^{13}$C, $^{19}$F, $^{31}$P, $^{15}$N, $^{17}$O, $^{11}$B, and $^{29}$Si NMR databases. AssignIt’s easy-to-use interface allows quick database information input, such as peak shift assignments, intensities, coupling constants, and multiplicities—all linked to chemical structure.

**Key Features**

- Import of a wide variety of NMR formats
- Assign atoms to peaks in the experimental spectrum
- Interactive coupling calculation tool
- Automated calculation of J value within a multiplet signal
- "Find signals with same J" feature to find similar splitting within a spectrum
- Intuitive interface with summary view and data-entry forms to add/edit assignments
- Automated and manual peak picking tools
- Full integration with DrawIt™ (structure drawing) and MineIt™
Advanced IR & Raman Functional Group Analysis

**Interpret a Spectrum:** Simply load a spectrum and click a peak of interest; Analyzelt then lists all functional groups possible at that peak position. Compare peak regions for each group by overlaying with the spectrum and narrow results by tagging the “most likely” candidates.

**Correlate a Structure with a Spectrum:** This powerful feature helps determine if a proposed structure matches an observed spectrum. Just draw or import a structure to view its component functional groups. Then compare peak regions for each group by overlaying with the spectrum.

**Build Your Own Knowledgebases:** Improve interpretations by building knowledgebases of functional groups to use with Analyzelt’s knowledgebase.

**Benefits**
- Useful in identification of spectra of unknown compounds
- Useful in classification/pattern characterization of chemicals
- Supplemental to other methods of spectral interpretation

**Key Features**
- Knowledgebase of over 200 functional groups and hundreds of interpretation frequencies
- Import and peak analysis of spectra
- Intelligent “Suggest a Peak” feature
- Determine if a structure matches a spectrum
- Browse knowledgebase by chemical class
- Tag and summarize negative or positive interpretations
- Peak overlay display for easy comparison
- Display/highlight structural bonds involved in vibrational frequency
- Build your own knowledgebase to use in analyses
- For those expert and non-expert in spectral interpretation
- Link to additional data in Sadtler Handbook (AnalyzeIt IR only)
Advanced IR Polymer Functional Group Analysis

Simply load a spectrum and click a peak of interest; Analyzelt then lists all functional groups possible at that peak position. Compare peak regions for each group by overlaying with the spectrum and narrow results by tagging the “most likely” candidates.

Benefits
• Useful in the identification of IR spectra of unknown polymers
• Useful in classification / pattern characterization of polymers
• Supplemental to other methods of spectral interpretation

Key Features
• Knowledgebase of 100 functional groups and hundreds of interpretation frequencies
• Import and peak analysis of spectra
• Intelligent “Suggest a Peak” feature
• Tag and summarize negative or positive interpretations
• Browse knowledgebase by chemical class
• Peak overlay display for easy comparison
• Display / highlight structural bonds involved in vibrational frequency
• View notes for functional groups when available
• Build your own knowledgebases to use in analyses
• For those expert and non-expert in polymer interpretation
Reliable NMR Spectrum Prediction

With PredictIt NMR, perform database-based NMR spectrum predictions for $^{13}\text{C}$, $^{1}\text{H}$, and other nuclei.

Predictions are performed automatically when users open a structure in PredictIt NMR. To make predictions, this tool examines databases of substructures that have $^{1}\text{H}$, $^{13}\text{C}$ or other shifts assigned to them. The substructures are defined by the number of shells that represent atoms within n bonds of the central atom.

For example, a shell of four would include the central carbon atom and all atoms within four bonds of this atom. After looking for exact matches, PredictIt NMR looks for matching shells for each atom in the structure, starting with shell four and proceeding to smaller shells until matches are found.

The tool searches the database(s) for specific chemical environments, which are described by a modified HOSE (Hierarchically Ordered Spherical description of Environment) code, a topology code used to describe the chemical surroundings of an atom in a molecular structure. The original structure and results are displayed in PredictIt NMR’s main window. Each atom’s average shift (and standard deviation) is displayed at the top level of the tree control.

Solvent-Specific Prediction for Improved Accuracy

KnowItAll offers the first solvent-specific NMR chemical shift prediction on the market. Users can choose from a list of common solvents such as chloroform, acetone, and dimethyl sulfoxide and KnowItAll will automatically recalculate all chemical shifts for that solvent.

More Than Just the Spectral Data

Predicted peak shifts are not the only piece of information that NMR spectroscopists need. PredictIt NMR not only allows easy retrieval of the real spectral data used to build the prediction, but also access to available information related to the reference spectrum, such as sample source, solvent, conditions of production, equipment, and properties for the molecule.
ProcessIt™ IR provides a variety of tools to process spectra and improve the quality of archived data and search results. It can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to ProcessIt IR to correct potential searching problems and transferred back.

**Processing Capabilities Include:**
- Flatline
- Truncation / Padding
- Normalization
- Smoothing (Quad-Cubic Savitsky Golay, Fourier methods)
- Baseline Correction (spline, linear, and polynomial methods)
- ATR Correction
- Reverse ATR Correction
- Kubelka-Munk Transform
- Spectral Subtraction and Spectral Addition
- Avererage Spectra
- Peak Picking

**Analysis Capabilities Include:**
- Area Under the Curve (AUC)
Raman Spectrum Processing

ProcessIt Raman provides a number of tools to process spectra and improve the quality of archived data and search results. It can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to ProcessIt Raman to correct potential searching problems and transferred back.

**Processing Capabilities Include:**
- Flatline
- Truncation / Padding
- Normalization
- Derivative
- Smoothing (Quad-Cubic Savitsky Golay, Fourier methods)
- Baseline Correction (spline, linear, and polynomial methods)
- Spectral Subtraction and Spectral Addition
- Average Spectra
- Peak Picking

**Analysis Capabilities Include:**
- Area Under the Curve (AUC)
Mass Spectrum Processing

ProcessIt™ MS can be used to import and open GC/MS and LC/MS files and view and select MS scans within them. Selected MS scans can be added to user databases and searched. It also enables users to perform spectral averaging and subtraction and viewing of selected ion chromatograms (SICs). It supports MS and hyphenated data from more than 40 common file formats.

Spectral Subtraction

This feature allows calculation of the average mass spectrum from several scans and also allows the elimination of background noise via manual background subtraction. Single or multiple ranges for either process can be specified.

Selected Ion Chromatograms (SICs)

ProcessIt™ MS allows the display of a selected ion chromatogram in a different color. Multiple ion chromatograms can be displayed in the first pane. A selected ion chromatogram is very useful feature for verifying target molecules and determining whether the background profile is constant during the entire run.
NMR Spectrum Processing

With ProcessIt NMR, import and process NMR spectra from various sources to improve the quality of archived data and search results. This tool is easy to use, yet offers a comprehensive set of processing features to correct experimental artifacts and improve the appearance of your spectra.

Chemists and spectroscopists can use ProcessIt NMR at their own desktops to process and re-process experimental data. In addition to being more convenient for the user, ProcessIt also saves valuable processor time at the instrument, thereby improving sample throughput.

Because ProcessIt NMR is fully integrated in the KnowItAll informatics environment, processed spectra can be transferred to other KnowItAll tools with a single click.

Key Features
- Import 1D processed or FID spectra from multiple formats
- Processing features: zero filling, interactive window functions, and Fourier transform
- Automatic and manual phase correction
- Automatic and manual baseline correction, includes polynomial, spline and linear algorithms
- Automatic and manual peak picking
- Automatic and manual integration
- Addition and subtraction of spectra
- Overlay multiple spectra for easy comparison
- Macro capability for quick and efficient processing
- Export in JCAMP format
- Spectrum handling tools, such as horizontal zoom, box zoom, hand cursor, and scaling
- Integrated with MineIt for archiving of processed spectra, ReportIt to create reports containing spectra, peak, and integral tables, and SearchIt for spectral searches
ChemWindow is the software chemists worldwide choose for chemical structure drawing. And now it’s included with the KnowItAll Analytical Edition!

ChemWindow provides an advanced set of drawing tools — just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

**Key Features**
- Customizable toolbars with tools to draw chemical structures, including bonds, rings, atom labels, charges, etc.
- Chemical recognition features such as hot keys, chemical syntax checker, tools to calculate mass and formula, etc.
- Advanced stereochemical recognition—using technology not available in other packages.
- OLE (Object Linking and Embedding) technology for in-place editing in word processing and presentation software
- Predefined styles for captions and structures
A Full-Featured Publishing Program

With ReportIt, create standard reports, design papers, presentations, and web publications that include annotations, tables of data, spectra, 2D and 3D structures, and more.

Key Features

- Custom templates to create uniform reports for enterprise-wide format standardization
- Customizable toolbars to draw chemical reactions and other reports, including arrows, text boxes, shapes, etc.
- Clip art libraries with hundreds of laboratory glassware drawings and engineering symbols
- OLE technology (Object Linking and Embedding) for in-place editing in word processing and presentation software
- MS fragmentation tool to display a mass for each fragment
- Advanced editing options to align, space, center graphics, and rotate captions
- Predefined styles for captions and structures
- 3D structure visualization for high-quality, realistic 3D drawings
- Table tool to enter and organize your data
- Spectrum / chromatogram import in common native file formats
- Multi-spectrum display in three display modes: overlay, stack, and offset
- Advanced spectrum display editing features to customize the appearance of spectra and chromatograms, including axes, colors, labels, etc.
- Custom annotation tool to link objects like spectral peaks to text graphics or chemical structure captions

Web Training Resources

BrowseIt is a web browser built into the KnowItAll software with links to KnowItAll tutorial videos and other resources for KnowItAll users.
KnowItAll Spectral Libraries (Optional)

Bio-Rad is the leading producer and publisher of fully verified spectral databases, with a collection that contains over 2.5 million spectra (IR, Raman, NIR, NMR, MS, and UV-Vis) covering pure compounds and a broad range of commercial products. By combining KnowItAll Spectral Libraries with the award-winning KnowItAll software, Bio-Rad offers a complete, unified solution for spectroscopy that is unparalleled.

These spectral collections are extremely useful when trying to identify or classify unknown spectra. Whether users need access to polymers, pure organics, inorganics, organometallics, or industrial compounds within application areas such as Pharmaceuticals, Forensics, and Material Sciences, users can be certain that this collection will meet their needs.
Multivariate Processing Made Simple

AnalyzeIt™ MVP, which incorporates Infometrix' chemometrics technology for principal component analysis (from the well-known Pirouette® software), provides a powerful tool for expert and nonexpert users alike to perform multivariate analysis of spectroscopic, chromatographic, or numeric data.

Benefits

- Gain insight into hidden patterns / relationships in data
- Explore data correlations to answer critical research, development, or production questions
- Store results for future reference, reporting, investigation

Comprehensive Chemometrics Modeling Software

Infometrix designed and developed the Pirouette software over 25 years ago to address the need for a tool to organize and understand complex data. The software balances the necessary algorithmic requirements with a simple user interface and is used for:

- Data mining, visualization and organization
- Classification analysis to identify the origin of a sample
- Quantitative analysis to estimate a concentration or other property that is hard to measure more directly
- Unmixing signals to identify and apportion the component parts of a mixture

What is Multivariate Analysis?

Multivariate analysis (including principal component analysis, PCA) refers to the statistical analysis techniques where multiple variables are analyzed to determine the contribution made by each variable to an observed result. This permits patterns to emerge from within the data. Researchers can use this method of analysis to examine quantitative data in more depth than from a basic cross-analysis of the data.