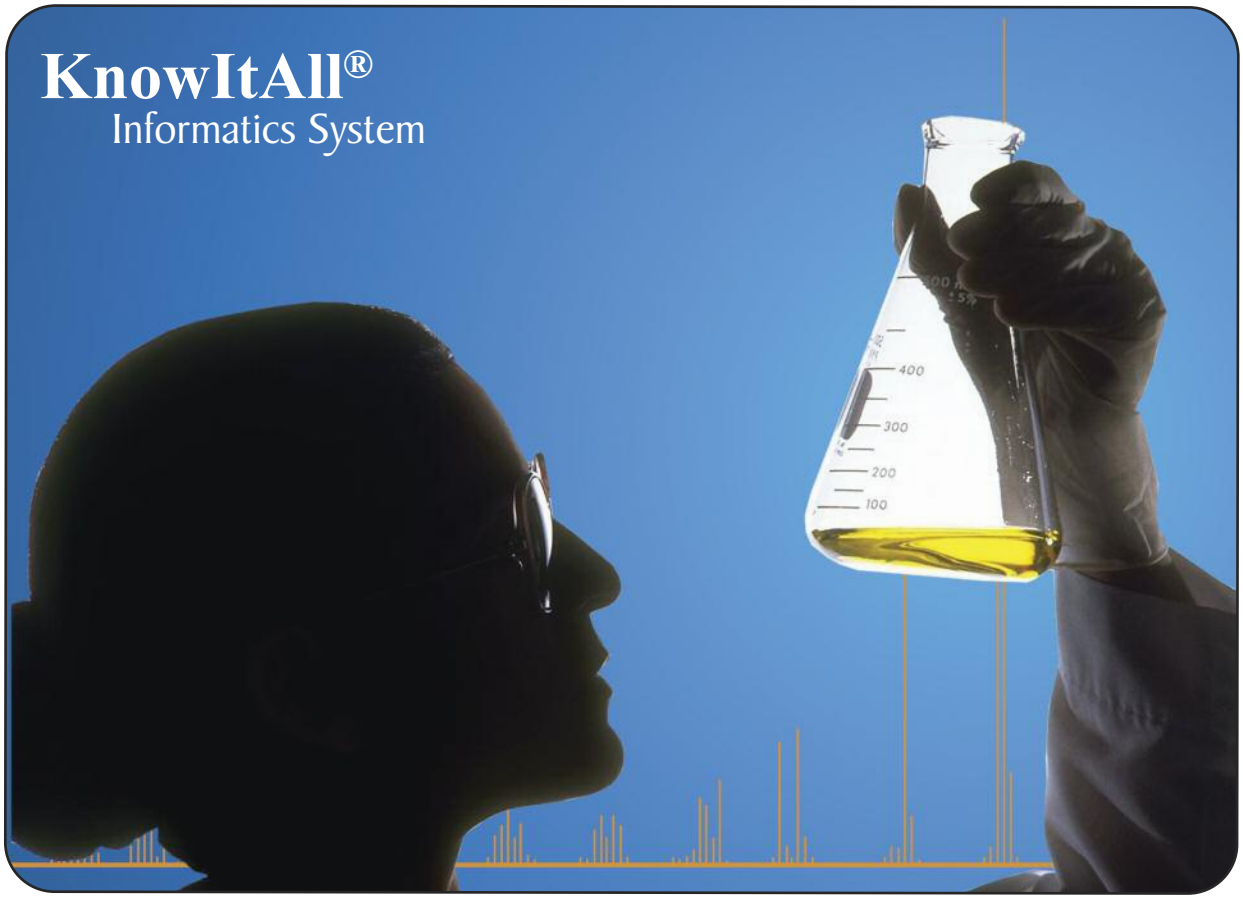

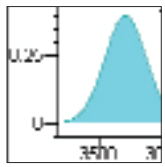

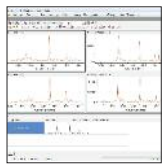

Analytical Edition

IR, Raman, NMR, NIR, MS, UV-Vis, Chromatography

BIO-RAD

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e-mail: sales@madatec.com

Spectroscopy Software for Multiple Techniques

The award-winning KnowItAll Informatics System, Analytical Edition offers a unique interface for spectroscopists. By integrating multiple types of analytical data (**IR, Raman, NMR, NIR, MS, UV-Vis, chromatograms**), chemists can perform multiple tasks in relationship to that data—and ultimately extract greater knowledge from it.

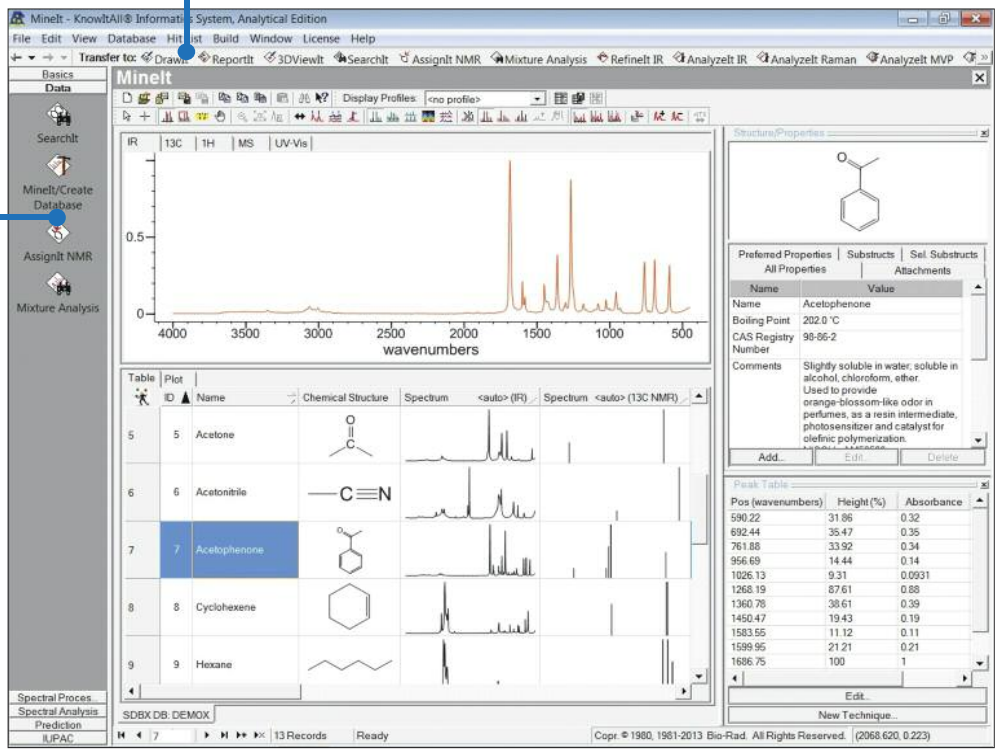
- **Spectral Searching, Processing & Analysis**
- **Data Management**
- **Structure Drawing & Reporting**

True Integration.
Instantly transfer data from one application to another.

Integrated Informatics.
Manage and communicate spectroscopic, chemical, and analytical information.

Versatile Toolboxes.
Easily evaluate spectroscopic and analytical data with a suite of informatics applications.

Desktop & Enterprise Solutions.



How the Interface Works: *The KnowItAll interface is designed so the user can 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. Multiple tasks are performed using logically grouped "**toolboxes**." Because all the tools are located in a single, integrated environment, using this system will invariably save time and improve workflow. Ultimately, by combining tools and data into one system, the end result is greater ability to extract knowledge from data.*

VIEW DEMO MOVIES

See KnowItAll in action at www.training.knowitall.com

What is in this Edition?

The KnowItAll Analytical Edition offers the following tools and options.

Data Toolbox

SearchIt™	Database searching (full spectrum, structure, peak, property, etc.)
MineIt™	Data display and mining
Database Building	Build multi-technique databases with spectra and structures
Overlap Density Heatmap	Patented technology for visual datamining and analysis
Batch Property Calculation	Calculate properties for entire databases
AssignIt™ **NMR**	Add assignments to NMR databases
Mixture Analysis	Analyze experimental spectral data of mixtures

Spectral Processing Toolbox

RefineIt™ **IR**	IR spectrum processing
RefineIt™ **Raman**	Raman spectrum processing
ProcessIt™ **NMR**	NMR spectrum processing
ProcessIt™ **MS**	MS and hyphenated MS processing

Spectral Analysis Toolbox

AnalyzeIt™ **IR** (optional)	IR spectral interpretation
AnalyzeIt™ **Raman** (optional)	Raman spectral interpretation
AnalyzeIt™ **MVP** (optional)	Multivariate processing for chemometrics
ValidateIt™	Statistical model validation
AnalyzeIt™ **Polymer IR** (optional)	IR spectral interpretation for polymers

Prediction Toolbox

PredictIt™ **NMR**	NMR chemical shift prediction

Basics Toolbox

DrawIt™	2D structure drawing
ReportIt™	Publish professional reports, with structures, spectra, chromatograms, etc.
3DViewIt™	Visualization of 3D structures
BrowseIt™	Web portal with links to training resources and product news

Optional Solutions

In addition to the tools and options above, here are some other solutions available with KnowItAll Analytical Edition:

Spectral Databases	High-quality reference spectra for IR, Raman, NMR, NIR, MS, UV-Vis, including Sadtler™ spectra
Infometrix Pirouette Software	Additional chemometrics tools for classification, data exploration, and multivariate regression
IUPAC DrawIt™	Convert IUPAC name to structure
IUPAC NameIt™	Convert structure to systematic IUPAC name
KnowItAll® **Enterprise Server**	Centralize spectral and chemical information on the KnowItAll server
Upgrade Plan	Support and upgrade plan for KnowItAll users

Data Toolbox

SearchIt™

Database Searching

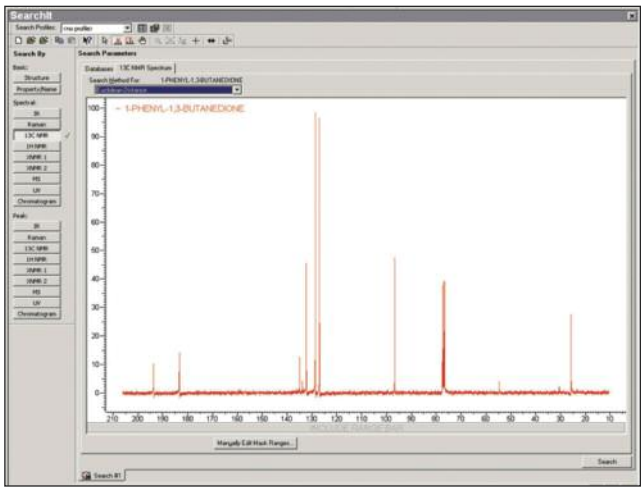
SearchIt allows users to import data and search against KnowItAll user-generated or reference databases. Searches are fully customizable and are driven by powerful algorithms. Searches can be performed by name, structure, substructure, properties, and analytical data (including spectra)—in any combination.

Multi-Technique Spectral Searching

Using Bio-Rad's unique multi-technique searching technology, the KnowItAll environment 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, a user can query an NMR spectrum in one database and a mass spectrum in another database at the same time and find the most relevant hits from each database, linked to one another by chemical structure.

Advanced Spectral Searching

SearchIt permits both full spectrum searching, 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.



MineIt™

Database Viewing & Mining

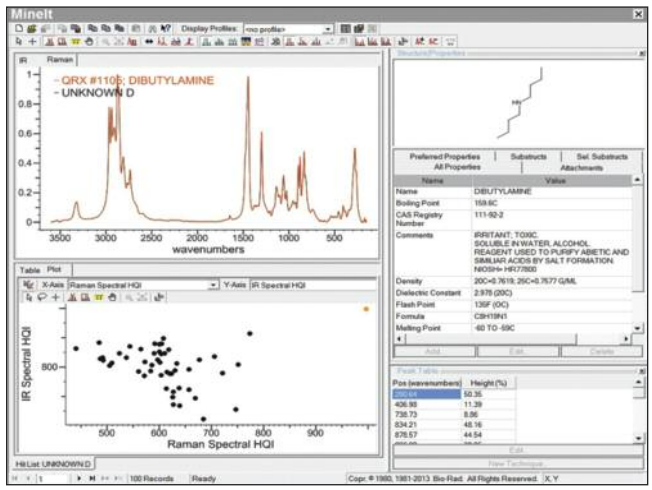
With MineIt, users can view reference databases, user-created databases, or search results.

Access Data from Multiple Techniques

The unified KnowItAll environment includes a powerful feature that allows the user to 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 analytical 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. Selecting any point on the scatter plot displays the compounds associated with that record.



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 Indicies - HQIs) against each other (e.g., IR HQI versus Raman HQI).

Database Building (*Feature in MineIt*)

Spectral Data Management

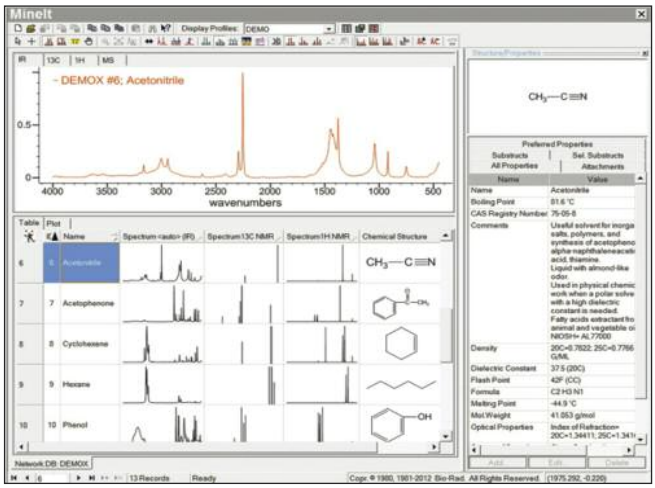
Chemists and spectroscopists produce valuable data every day within their organizations. Because Bio-Rad Informatics Division's primary business is creating spectral databases, we have built our KnowItAll solutions through years of experience in doing just that—building databases.

With KnowItAll's Database Building option, 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.

Features & Benefits

Centrally Store & Share Spectral & Chromatographic Data*

- Build databases with one or more techniques (NMR, MS, IR, NIR, Raman, UV-Vis, chromatograms)
- 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 (over 70 formats supported) 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



- Quick peak assignment for structures
- "Auto-Property" computes values such as formula, molecular weight, etc. on entire datasets
- Make database more powerful by adding spreadsheets, MSDS, and other documents or 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
- Share structure and property data for records in the database to increase productivity and avoid errors
- Deploy in a single laboratory or globally throughout an entire organization
- Databases can be stored on the desktop or on an enterprise server for maximum speed and security in data sharing

Customize & Protect Databases

- Databases can be customized to meet each laboratory's specifications
- Users can create custom fields to support associated metadata relevant to their work
- Choose from three types of property fields: text, numeric, and hyperlink
- Generate "preferred property" forms so users enter properties consistently throughout an organization
- Set spectral parameters such as x- and y-resolution
- Manage access privileges
- Password protect data

Extract the Most Information from Your Data

- Fully integrated with other KnowItAll applications for processing, database searching/mining, analysis, structure drawing, processing, reporting, and more

** Types of data accessible using MineIt will depend on the "edition" of KnowItAll and options licensed, databases licensed, etc. For example to access spectra from multiple spectral techniques, you would need to have a KnowItAll edition that supports multiple spectral techniques.*

Overlap Density Heatmap

(Feature in MineIt)

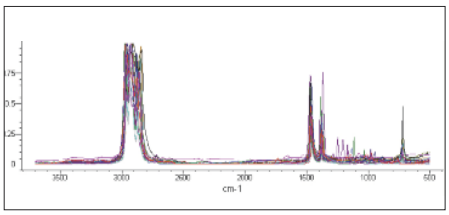
Patented Technology for Visual Data Mining & Analysis

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.

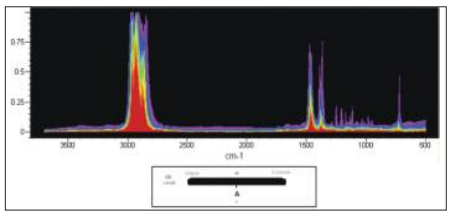
Traditional Stacked Display

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



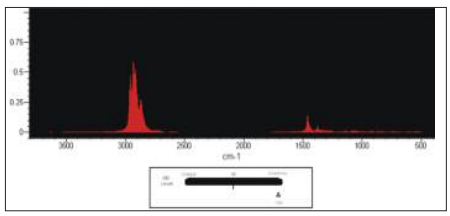
OD Heatmap OD Level = 0

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.



OD Heatmap OD Level = 100

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



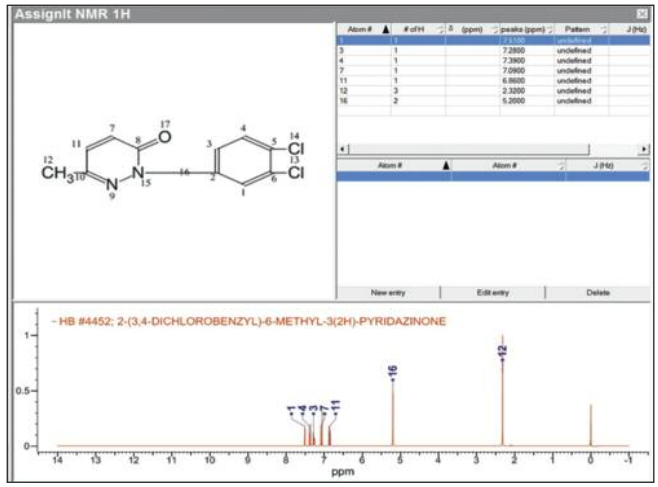
AssignIt™ NMR

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 the Database Building Option

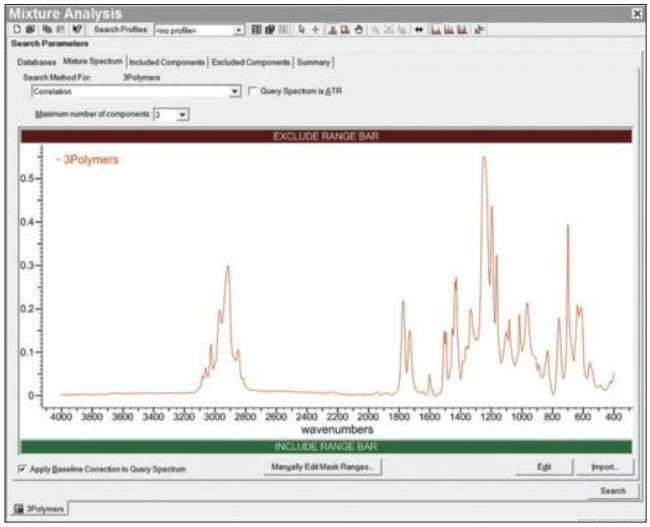


Mixture Analysis

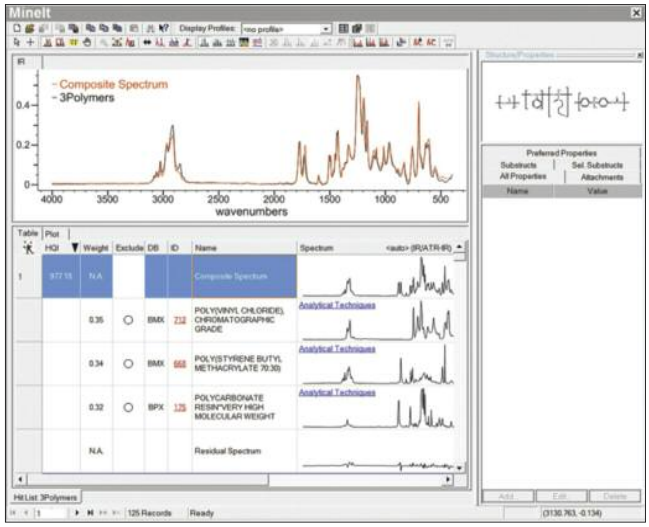
Analyze Experimental Spectral Data of Mixtures

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.



A mixture spectrum is imported and analyzed against reference spectral databases.



Results show possible components in the mixture.

Spectral Processing Toolbox

RefineIt™ IR

IR Spectrum Processing

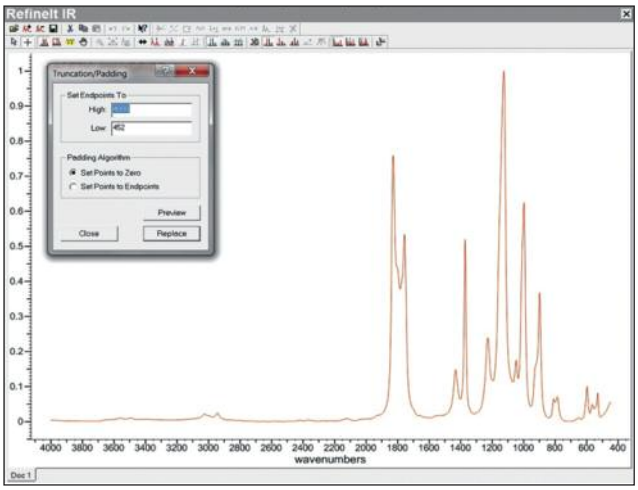
RefineIt IR provides a variety of tools to process spectra and improve the quality of archived data and search results. RefineIt IR can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to RefineIt IR to correct potential searching problems then 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
- Peak picking

Analysis Capabilities Include:

- Area Under the Curve (AUC)



RefineIt™ Raman

Raman Spectrum Processing

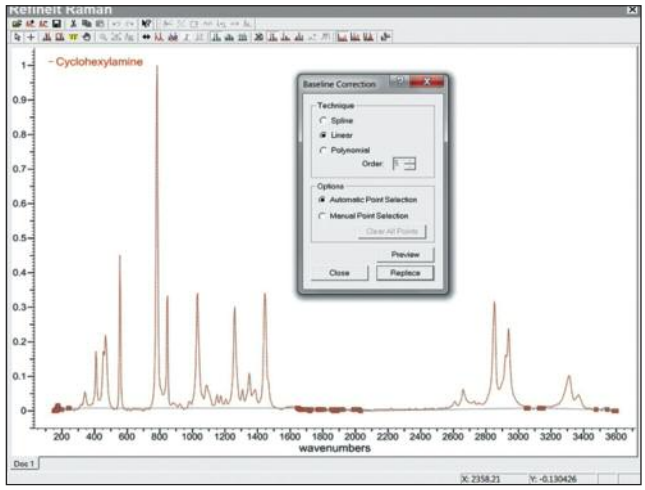
Like RefineIt IR, RefineIt Raman provides a number of tools to process spectra and improve the quality of archived data and search results. RefineIt Raman can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to RefineIt Raman to correct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

Processing Capabilities Include:

- Flatline
- Truncation/Padding
- Normalization
- Smoothing (Quad-Cubic Savitsky Golay, Fourier methods)
- Baseline correction (spline, linear, and polynomial methods)
- Spectral subtraction and spectral addition
- Peak picking

Analysis Capabilities Include:

- Area Under the Curve (AUC)



ProcessIt™ NMR

NMR Spectrum Processing

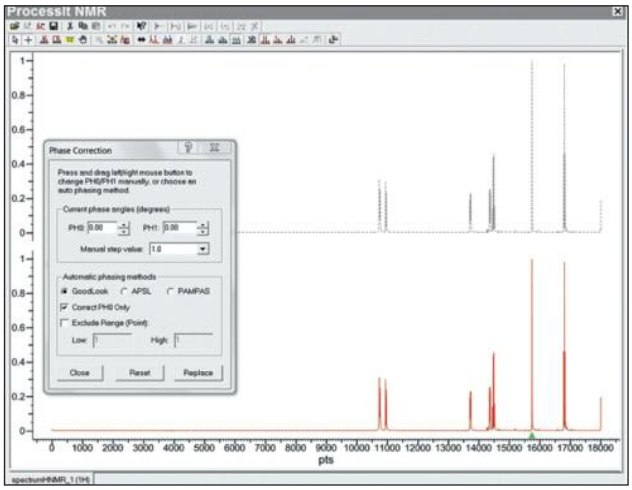
With ProcessIt NMR, import and process NMR spectra from various sources to improve the quality of archived data and search results. This tool is easy to use, yet offers a comprehensive set of processing features to correct experimental artifacts and improve the appearance of your spectra.

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



ProcessIt™ MS

Mass Spectrum Processing

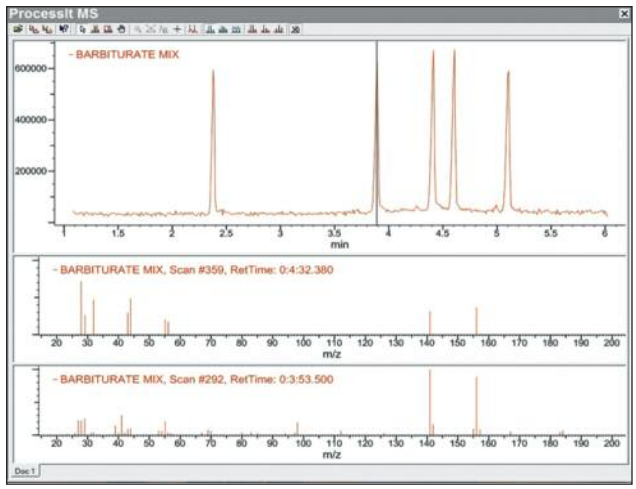
ProcessIt MS can be used to import and open GC/MS and LC/MS files and view and select MS scans within them. Selected MS scans can be added to user databases and searched. It also enables users to perform spectral averaging and subtraction and viewing of selected ion chromatograms (SICs). It supports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



Spectral Analysis Toolbox

AnalyzeIt™ IR & Raman

(*Optional*)

IR & Raman Spectral Interpretation

Interpret a Spectrum

Simply load a spectrum and click a peak of interest; AnalyzeIt 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 structure matches a 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

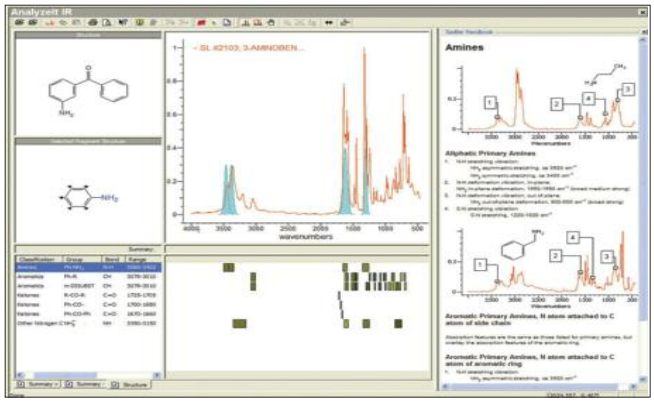
Improve interpretations by building knowledgebases of functional groups to use with AnalyzeIt’s knowledgebase.

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)



AnalyzeIt™ MVP

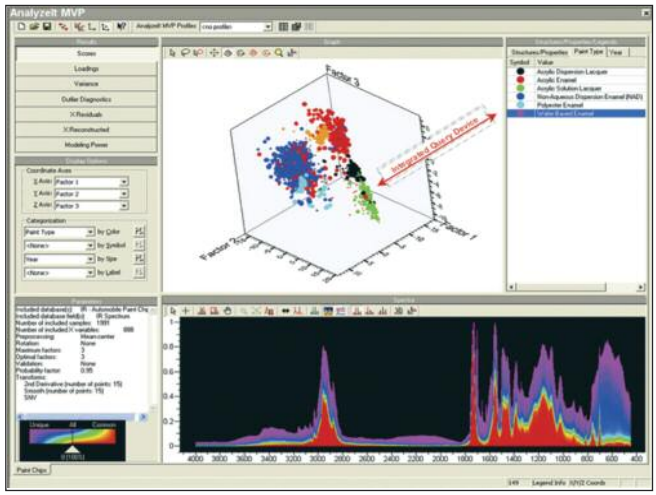
(*Optional*)

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



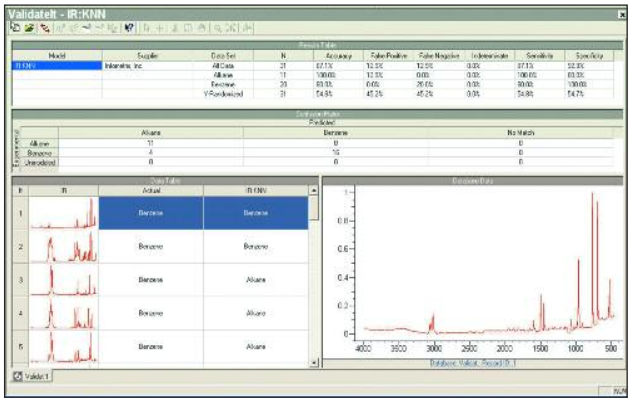
What is Multivariate Analysis? *Multivariate analysis (including principal component analysis, PCA) refers to the statistical analysis techniques where multiple variables are analyzed to determine the contribution made by each variable to an observed result. This permits patterns to emerge from within 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.*

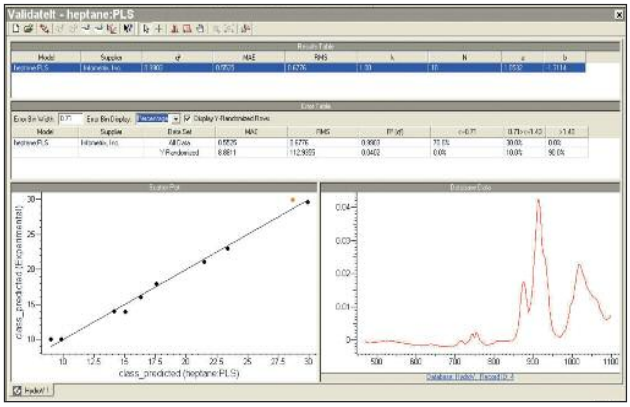
ValidateIt™

Predict & Validate by Spectrum/Chromatogram

If AnalyzeIt MVP option is available, one can use chemometric models to predict properties of a sample from the spectrum or chromatogram. With ValidateIt, a user can test a model's performance statistically before deploying it in a production environment.

For a categorical model, accuracy, false positive, false negative, sensitivity, and specificity are calculated. The confusion matrix is presented along with a table of experimental vs. predicted measurements. For a regression model, q^2, RMS, and MAE are calculated, and one can set a bin value to group results.





AnalyzeIt™ Polymer IR

(Optional)

Interpret IR Spectra of Polymers

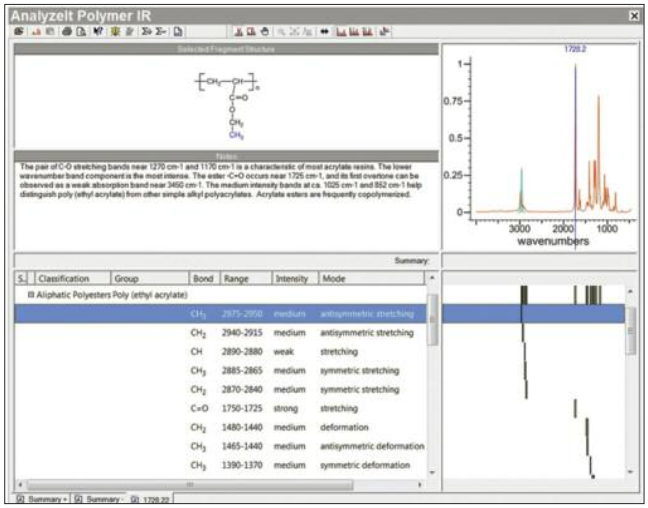
Simply load a spectrum and click a peak of interest; AnalyzeIt then lists all functional groups possible at that peak position. Compare peak regions for each group by overlaying with the spectrum and narrow results by tagging the “most likely” candidates.

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



Spectral Prediction Toolbox

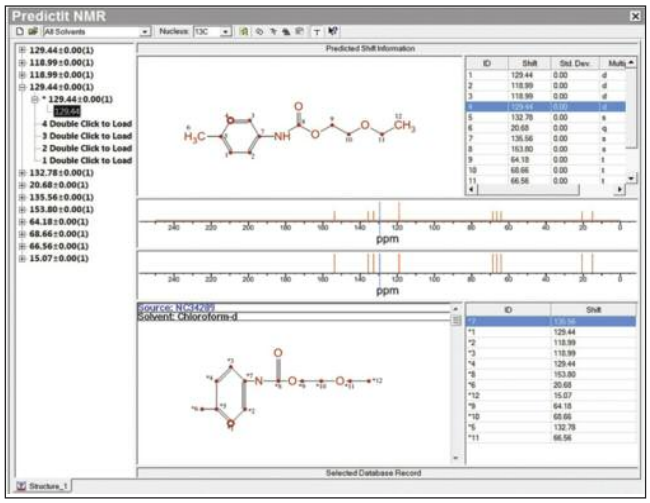
PredictIt™ NMR

Reliable NMR Spectrum Prediction

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

Predictions are performed automatically when you open a structure in PredictIt NMR. To make predictions, this tool examines databases of substructures that have ^{1}H, ^{13}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.

Basics Toolbox

DrawIt™

A Full-Featured 2D Structure Drawing Program Using ChemWindow® Technology

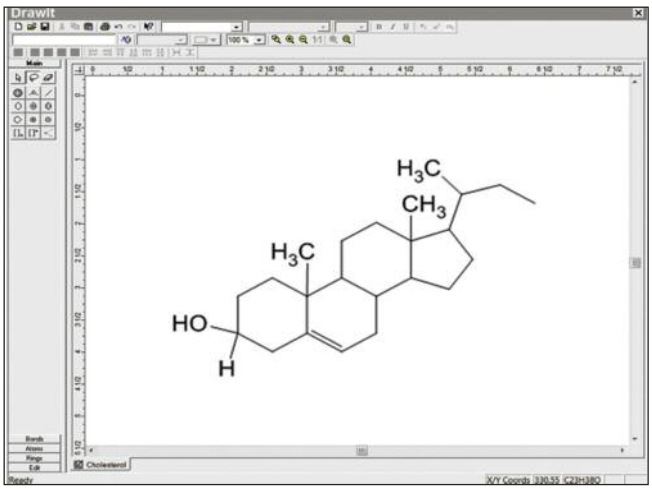
DrawIt provides an advanced set of drawing tools — just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

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.
- Stereochemical recognition including R/S and E/Z isomers
- OLE (Object Linking and Embedding) technology for in-place editing in word processing and presentation software
- Predefined styles for captions and structures

Easily Import Existing Structures

For customers using ChemDraw, files can be imported directly into DrawIt. For those using ISIS/Draw, exported MOL files can also be imported. Many other file formats are also supported.



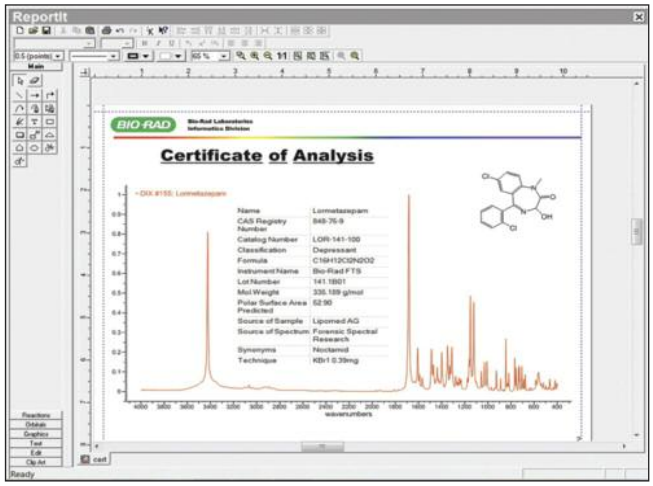
ReportIt™

A Full-Featured Publishing Program Using ChemWindow Technology

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

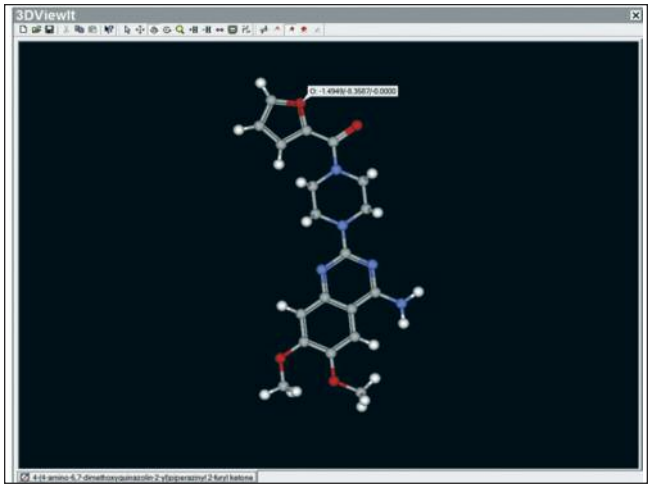
- Custom templates to create uniform reports for enterprise-wide format standardization
- Customizable toolbars to draw chemical reactions and other reports, including arrows, text boxes, shapes, etc.
- Clip art libraries with hundreds of laboratory glassware drawings and engineering symbols
- OLE technology (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 displays including 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



3DViewIt™

3D Structure Viewing

3D ViewIt allows the input of and visualization of 3D structures. A rudimentary 2D to 3D conversion is included for 2D structure files. The adjustable color display for atoms, bonds, and backgrounds provides high-quality, realistic 3D drawings, complete with spacefill, ball and stick, stick, and wireframe display options.



BrowseIt™

Integrated Web Resources

BrowseIt is a web browser built into the KnowItAll software with links to training resources, and product news.

Spectral Databases

Increase the Power of KnowItAll with Spectral Data

Bio-Rad is the leading producer and publisher of fully verified spectral databases, with a collection that contains over 1.4 million IR, Raman, NMR, NIR, , MS, and UV-Vis spectra covering pure compounds and a broad range of commercial products. By combining spectral reference databases 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.

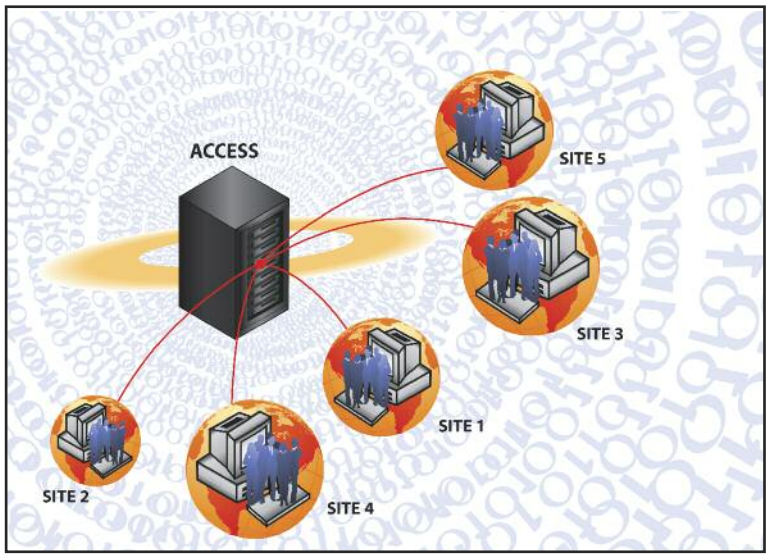
Bio-Rad offers the highest quality data on the market. Their rigorous qualifying procedures start at data acquisition and continue throughout the database development process. Most collections include the following features:

- Chemical and Physical Properties
- Chemical Structures
- Chemical Composition
- Sampling Technique
- Search-Optimized Database Architecture
- Data Authenticated by Independent Consultants

KnowItAll Desktop or Enterprise

Since it's introduction in 2001, the KnowItAll Informatics System software has been installed in thousands of laboratories as a convenient, highly-integrated desktop solution. Today, combined with the KnowItAll Enterprise Server technology, KnowItAll is a high performance and cost-effective solution for the entire organization. Suitable for deployment on virtually any scale—even globally—KnowItAll Enterprise Solutions can be the focal point for creating, storing, maintaining, and searching analytical data from an entire enterprise—all behind the security of the enterprise firewall.

Please ask for supplemental information about KnowItAll Enterprise Solutions and discover the advantages of elevating KnowItAll to the next level—the enterprise level.



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