KnowItAll®
Informatics System

www.knowitall.com

Analytical Edition

BIO·RAD

*Bio-Rad
Laboratories, Inc.*

BIO·RAD

One Solution

Improve Analysis, Data Management, & Workflow with the Proven Leader in Analytical Informatics

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 Solution.
Solve problems directly at the researcher's desktop

A Truly Unique Architecture to Manage Multiple Analytical Techniques & Tasks

The award-winning KnowItAll Informatics System, Analytical Edition offers the first, fully integrated software environment for analytical techniques such as IR, NMR, MS, UV/Vis, Raman, Near IR, and chromatographic data.

So now, researchers can finally have all the data and software solutions that they need in one place with:

- Analytical Data Management
- Spectral Processing
- Spectral Analysis
- Structure Drawing & Reporting
- Integrated toolsets to handle one or multiple analytical and spectroscopic techniques simultaneously!

Improve Workflow & Extract the Most Knowledge from Analytical Data

KnowItAll offers a truly unique single interface for spectroscopy and analytical research that seamlessly incorporates multiple types of analytical data and allows researchers to then perform multiple tasks in relationship to that data.

KnowItAll is designed so the user can 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. 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. And since there is only one interface, it is easy to learn and easy to use.

Ultimately, by combining all the tools and data that researchers need into one system, the end result is an even greater ability to extract knowledge from analytical data.

The Basics Application Toolbox

The Basics Application Toolbox offers all the tools needed to generate structures and reports. This toolbox also includes BrowseIt for access to a portal community designed specifically for KnowItAll users.

Basics
- DrawIt
- ReportIt
- 3DViewIt
- BrowseIt
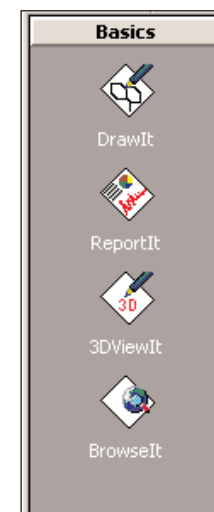
DrawIt™

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.

DrawIt features include:

- **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 Technology** or Object Linking and Embedding 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.
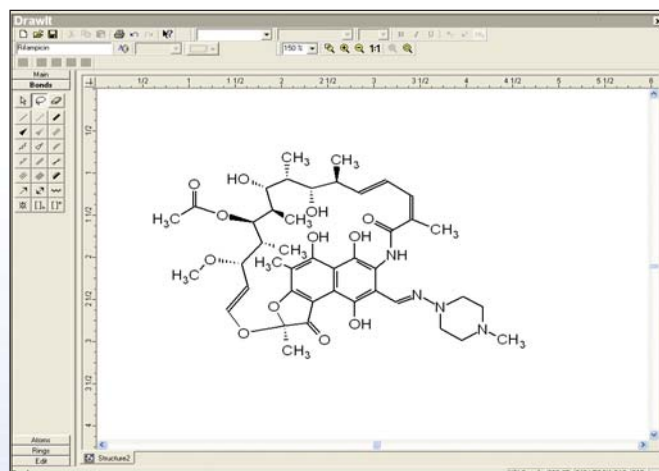
ReportIt™

A Full-Featured Publishing Program Using ChemWindow Technology

In addition to the most comprehensive structure drawing available, users can create standard reports, design papers, presentations, and web publications that fit specific communication needs to include annotations, tables of data, spectra, 2D & 3D structures, and more.

ReportIt features include:

- **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 office applications.
- **MS Fragmentation Tool** to display a mass for each fragment. Allows multi-fragmentation in one step.
- **Advanced Editing Options** to align, space, center graphics, and rotate captions.
- **Predefined Styles** for captions and structures.
- **3D Structure Visualization** for high-quality, realistic 3-D 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.
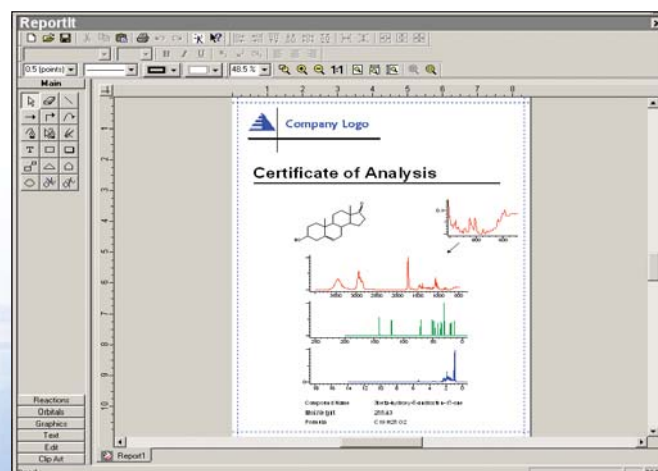
3DViewIt™

3D Structure Viewing

The 3D ViewIt application 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 & stick, stick, and wireframe display options.
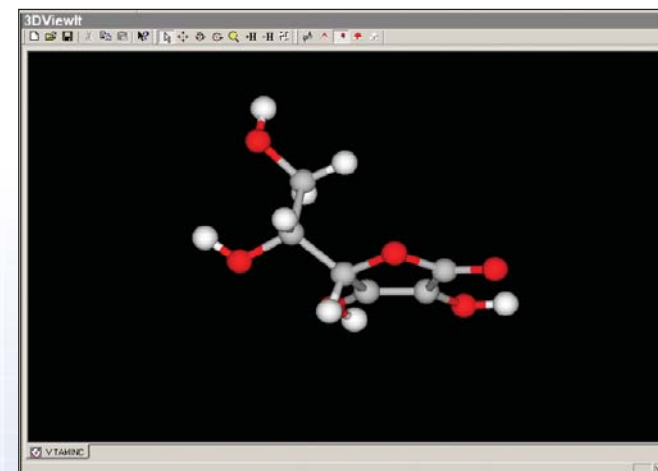
BrowseIt™

Integrated Web Resources

KnowItAll's BrowseIt™ application gives you access to a portal web community designed especially for KnowItAll users. This exclusive community offers tutorial movies, tips, application notes, and additional information.

The Data Application Toolbox

With the Data Application Toolbox, researchers can build, search, and mine user-generated or reference databases containing analytical (including spectra), chemical, and biological data.
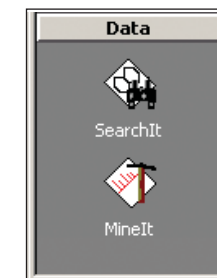
SearchIt™

Database Searching

The KnowItAll Analytical Edition allows you to import your own data and search against user-generated as well as reference databases. Searches are fully customizable and are driven by powerful, state-of-the art algorithms. Searches can be performed by name, structure, substructure, properties, and analytical data (including spectra)—in any combination.
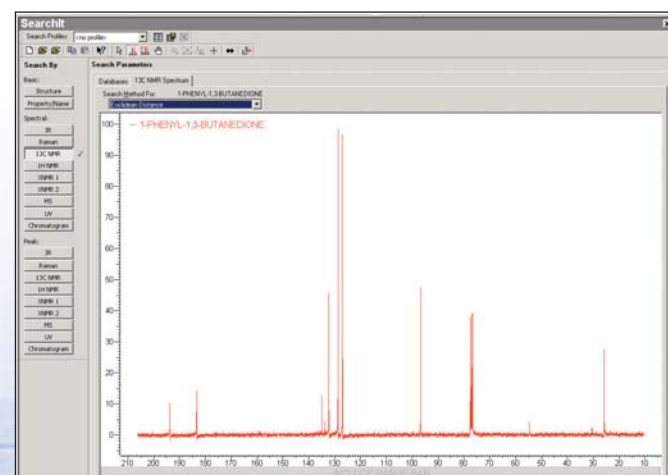
Multi-Technique Spectral Searching

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, as well as peak searching. Euclidean Distance, First Derivative Euclidean Distance, and Correlation algorithms are available for full-spectrum searches, and baseline correction is also available. For peak searches, the user can manually select peaks or use the automated peak picking capability.

Automated peak searching allows the user to specify the minimum intensity and maximum noise thresholds to maximize peak picking results. Mass spectrum peak picking allows the user to specify the minimum intensity, minimum and maximum mass ranges, mass tolerance, and the mass above which hits in the reference database containing the specified mass will be eliminated from the hit list.

MineIt™

Multi-Technique Database Mining & Building Option

Easily mine and manage chemical, spectral, and biological data with MineIt™ and the Database Building Option. With these tools, researchers can build their own searchable and comparable databases including chemical structures, ADME/Tox properties, and multiple analytical techniques such as NMR, MS, IR, GC, Near IR, Raman, and UV/Vis.

Customize Databases

Create customized fields or "preferred property" forms, so users can enter properties in a consistent way and thus maintain the integrity of data throughout the organization. There is also the option to password protect data and manage access privileges.

Sophisticated Analytical & Structure File Import

With KnowItAll's database building tool, directly import analytical data such as NMR, MS, IR, GC, Near IR, Raman, and UV/Vis data from a wide range of native file formats for many common instrument makes and models. So even if a laboratory has instruments from multiple vendors, researchers can use KnowItAll to archive all supported data. Users can also import multiple structure format and display stereochemical bonds and identifiers. Software includes batch import and export for batch handling of spectra, structures, and property files.

Advanced Datamining Capabilities

MineIt includes sophisticated datamining capabilities that allow users to convert masses of uninterpretable data into actionable information. The unique, fully user-definable color coding and weighted scoring scheme allows users to rank-order their datasets according to the priorities of a particular project, and then readjust the scheme for different projects.
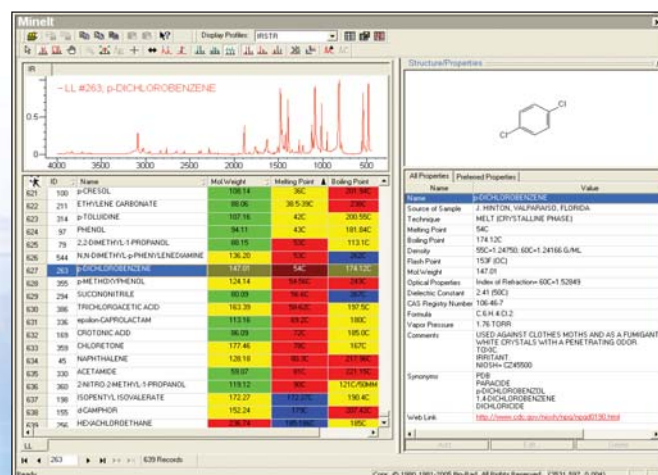
Overlap Density Heatmap

Patent Pending Technology for Data Mining & Analysis

Traditionally, the visualization of multiple spectra or chromatograms takes place in an overlay, offset, or stacked plot. These traditional plotting methods, however, obliterate trends when viewing large amounts of data.

Bio-Rad is pleased to announce a new breakthrough technology for visual data mining and analysis that can now turn these unmanageable amounts of data into actionable information. Part of the KnowItAll Analytical Edition, Overlap Density (OD) Heatmap and OD Consensus object technologies allow trends to be viewed with ease. Using these technologies, users can assess the similarities and dissimilarities in massive amounts of spectral, chromatographic, or other graphical data.

How Does It Work?

Specifically, Overlap Density Heatmaps allow the user to see the common features of the overlapped objects (such as spectra or chromatograms) by color coding spectral areas from highest to lowest overlap.

The OD Scale

An arbitrary scale was created to define the extent of overlap for the objects being compared and displayed:

OD Level	0	ALL	Shows all levels of object overlap
OD Level	100	COMMON	Shows only the areas of highest overlap
OD Level	-100	UNIQUE	Shows only the areas of lowest overlap

Controlling the Overlap Displayed: The OD Level Slider

The OD level can be changed with a single slider control to change the overlap density displayed in the OD Heatmap.
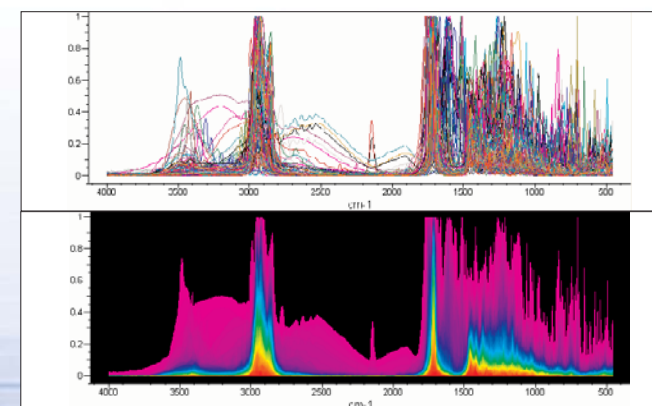
An OD Level = 0 will show all colors representing all overlap density levels; an OD level of 100 will show only red representing only those areas where 100% of the spectra share areas in common; and an OD level of –100 will show only violet areas representing only those areas where one spectrum exists but no other spectra overlap in the same area. Values in between display intermediate ranges of overlap.

### Overlap Density Consensus Spectra or Chromatograms

By tracing the outline of highest level of overlap, it is then possible to mathematically reconstruct a spectrum by using the maximum spectral y-values at each spectral x-value in the OD Heatmap. The resulting OD Consensus Spectrum can then in turn be used as the spectrum in a spectral search query to find similar spectra in databases.

For Application in Spectroscopy, Chromatography, Metabolomics, Chemometrics, & Beyond!

This technology can be used to analyze the large amounts of data from any analytical or chromatographic technique, including IR, NMR, MS, and Raman. It can be used in disciplines such as cheminformatics, metabolomics, chemometrics, genomics, and proteomics and has applicability in all branches of scientific research, including chemistry, life sciences, and diagnostics.

Traditional Stacked Display

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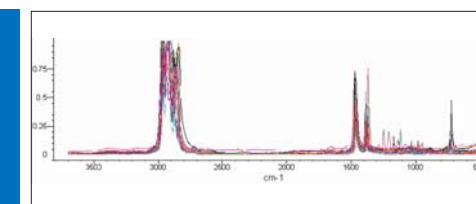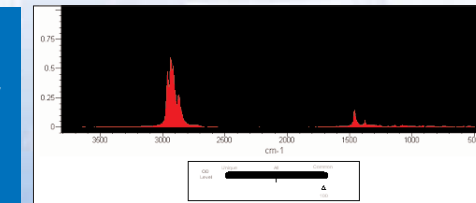

OD Heatmap OD Level = 0

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.
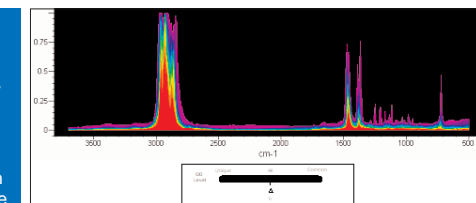
OD Heatmap OD Level = 100

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

The Spectral Processing Toolbox

The Spectral Processing Toolbox offers powerful spectral processing applications. These tools in combination with the spectral searching and database building tools in the Data Applications Toolbox offer a complete spectroscopic solution to meet your analytical needs.

CompareIt™

Data Plotting & Visualization

The CompareIt application is a powerful data analysis and visualization package built upon a cheminformatics software platform. With this application, researchers can visualize and compare numeric data within a single database or between multiple databases by building two-dimensional scatter plots.

Visualizing Data Trends

Any two data components from a dataset can be visualized, such as boiling point versus melting point; predicted water solubility versus experimental water solubility, and so on. For spectroscopists, CompareIt is extremely useful for plotting the results of spectral database searches from a sample run in multiple techniques. Visual analysis is easily achieved by plotting the quality of database matches (Hit Quality Indicies - HQIs) against each other, such as IR HQI versus CNMR HQI. Either axis can then be changed to introduce a third, fourth, or fifth technique into the evaluation. This simple plot greatly simplifies the interpretation of search results—because, in general, the "best hit" is the furthest from the origin, which may often NOT be the highest quality hit in one or the other technique alone.

Interpretability Beyond Traditional Spectral Searching

CompareIt can also enable the researcher to analyze trends revealed by visualization of chemical properties and separate data that follow a desired trend from that which does not. Selecting any point or group of points on the scatter plot will immediately display the compounds associated with that record, including a convenient view of all the data associated with the compound.
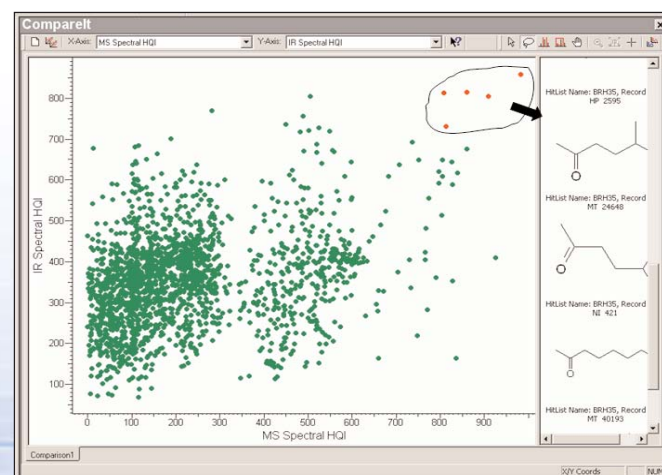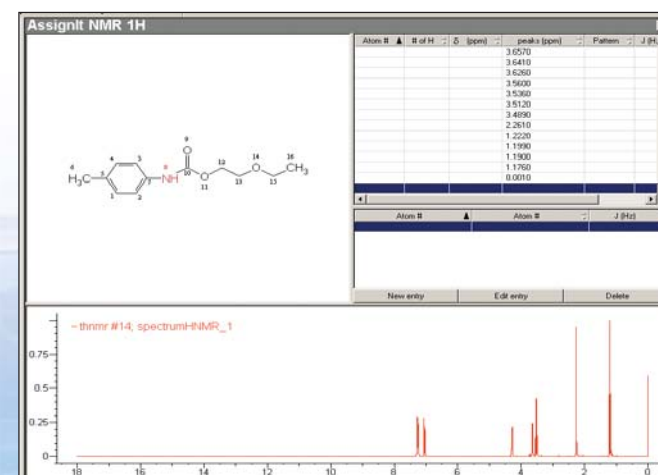
AssignIt NMR™
(Optional Application)

Create Fully Assigned NMR databases

AssignIt is an optional KnowItAll application that allows users to increase the value of the NMR databases they build. With the AssignIt application, users can 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 of AssignIt NMR include:

• 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.
• Publication-ready reports with spectra, structure, and coupling data.
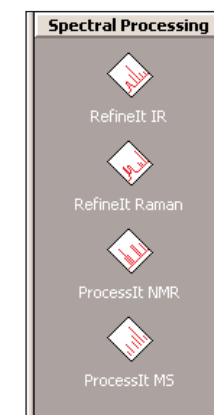
RefineIt™ IR

IR Spectrum Processing

RefineIt IR provides a variety of tools to process spectra and improve both the quality of search results and the overall look of publications. RefineIt IR can also be used in conjunction with other KnowItAll applications. For example, a spectrum can be transferred from the SearchIt™ application to RefineIt IR to correct potential searching problems then transferred back.

Processing capabilities of RefineIt IR include:

• Flatline
• Truncation/Padding
• Normalization
• Smoothing (Quad-Cubic Savitsky Golay, Fourier methods)
• Baseline correction (spline, linear, and polynomial methods)
• ATR correction
• Kubelka-Munk transform
• Spectral subtraction and spectral addition
• Peak picking
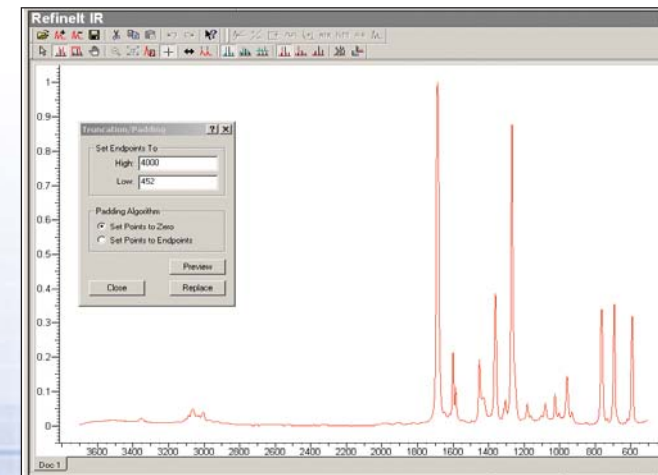
RefineIt™ Raman

Raman Spectrum Processing

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

Processing capabilities of RefineIt Raman 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

The Spectral Analysis Toolbox
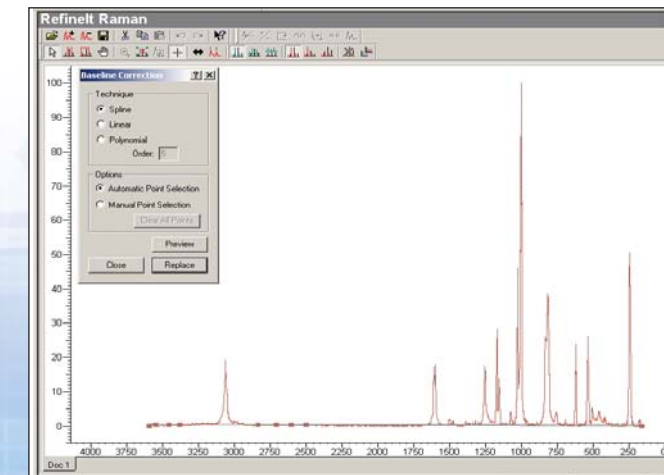
ProcesstIt™ NMR
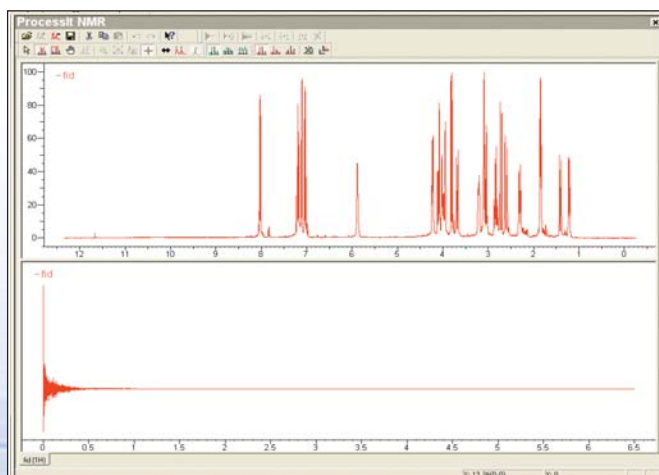**(Optional Application)**

NMR Spectrum Processing

ProcessIt NMR can seamlessly import and process NMR spectra from various sources to improve the quality of archived data and search results. This application 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 applications with a single click.

Features in ProcessIt NMR include:
- 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

The ProcessIt MS application 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 can be searched. In addition, the ProcessIt MS application enables users to perform spectral averaging and subtraction, and allows the viewing of selected ion chromatograms (SICs). ProcessIt MS can import MS and hyphenated technique data in more than 40 common file formats. This application provides the ability to view, select, and analyze MS scans within chromatographic runs.

Spectral Subtraction

The ProcessIt MS application allows the 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)

The ProcessIt MS application 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.
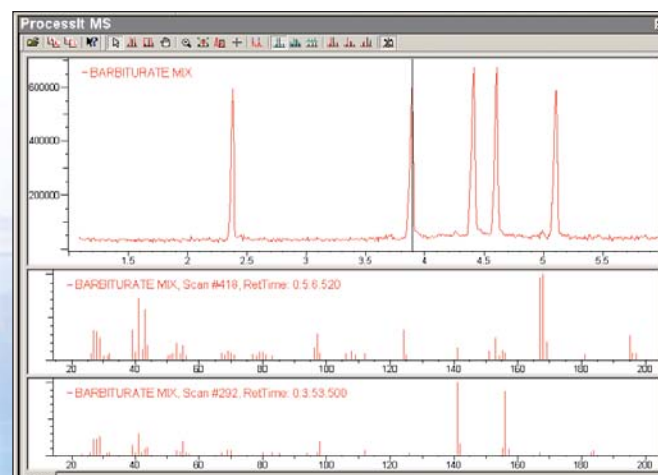
*The Spectral Analysis Toolbox offers several specialized tools to analyze spectra.*
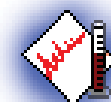
AnalyzeIt IR™
(Optional Application)

IR Spectrum/Structure Correlation

AnalyzeIt IR can be used to help interpret the bands in an infrared spectrum. Simply load a spectrum and click on a peak of interest to generate a list of all functional groups possible at that position. AnalyzeIt is also capable of suggesting the best peak to begin an interpretation. AnalyzeIt features over 200 functional groups and hundreds of interpretation frequencies.

AnalyzeIt IR also supports the ability to correlate from a structure, which helps to determine if a structure matches an IR spectrum. Simply draw a structure and AnalyzeIt will break the structure into its component functional groups to overlay with the spectrum.
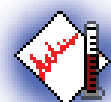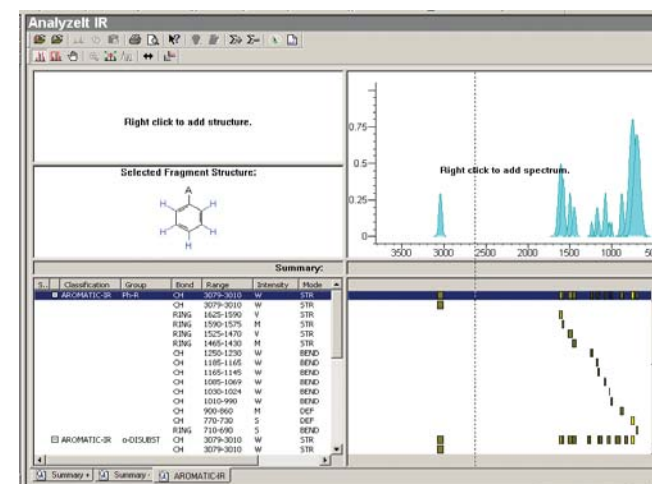

AnalyzeIt Raman™
(Optional Application)

Raman Spectrum/Structure Correlation

All of the same features found in AnalyzeIt IR are now available to Raman spectroscopists. Features such as browsing the knowledge base for functional group classes or summarizing your results are included. AnalyzeIt Raman features over 200 functional groups and hundreds of interpretation frequencies.

This application also provides the ability to correlate from a structure, a powerful feature that helps to determine whether a structure matches an Raman spectrum. Simply draw a structure and AnalyzeIt will break the structure into its component functional groups to overlay with the measured spectrum.
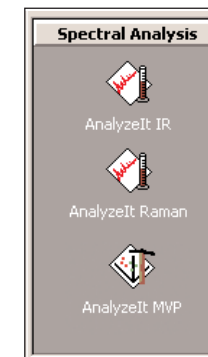
AnalyzeIt MVP™
(Optional Application)

Multivariate Processing Made Simple

The elegance and power of Infometrix Pirouette® chemometrics software are a perfect complement to the cheminformatics and comparitive visualization tools in the KnowItAll® system. The result is an advanced tool for multivariate processing to analyze spectroscopic chromatographic, or numeric data with efficiency and ease. This application offers experts users and non-expert users alike a powerful yet intuitive interface for multivariate processing that enables them to:

- Gain insight into hidden patterns and relationships in users' data
- Explore data correlations to answer critical research, development, or production questions
- Facilitate the storage of analysis results for subsequent reference, reporting, or investigation

What is Multivariate Analysis?

Multivariate analysis is a statistical analysis technique where multiple variables are analyzed separately to determine the contribution made by each variable to an observed result. It can examine quantitative data in more depth than can usually be obtained from a basic cross-analysis of the data. This permits patterns to emerge from within the data.
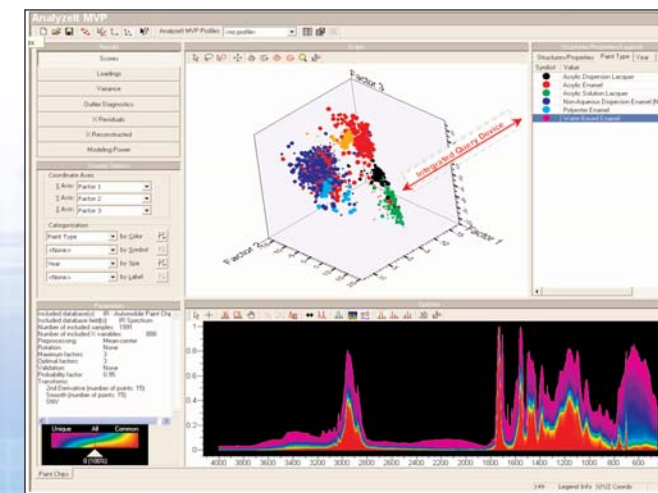
The Spectral Prediction Toolbox offers specialized tools for NMR prediction.

PredictIt NMR™
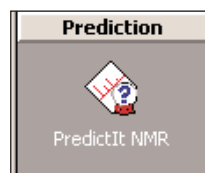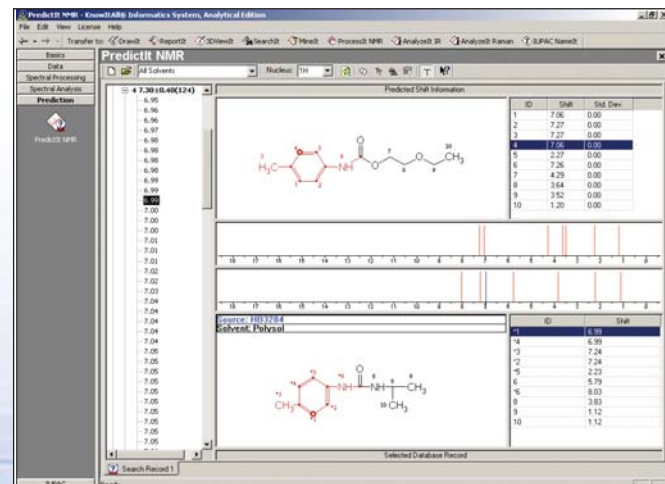
Reliable NMR Spectrum Prediction

With the PredictIt NMR application, database-based NMR spectrum predictions can be performed for ^{13}C, ^{1}H, and many other nuclei.

Predictions are performed automatically when you open a structure in the PredictIt NMR application. To make predictions, the application 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, the PredictIt NMR application looks for matching shells for each atom in the structure, starting with shell four and proceeding to smaller shells until matches are found.

The program 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.

Once the database has been examined, both 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's prediction application 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. The PredictIt NMR application not only allows easy retrieval of the real spectral data used to build the prediction, but also access all available information related to the reference spectrum, such as sample source, solvent, conditions of production, equipment, and properties for the molecule.

Basics Toolbox
- DrawIt
- ReportIt
- 3DViewIt
- BrowseIt

Data Toolbox
- SearchIt
- MineIt
- CompareIt
- Overlap Density Heatmaps
- Database Building (Optional)
- AssignIt NMR (Optional)

Spectral Processing Toolbox
- RefineIt IR
- RefineIt Raman
- ProcessIt MS
- ProcessIt NMR (Optional)

Spectral Analysis Toolbox
- AnalyzeIt IR (Optional)
- AnalyzeIt Raman (Optional)
- AnalyzeIt MVP (Optional)

Spectral Prediction Toolbox
- PredictIt NMR

Additional Software Options
- Annual Maintenance
- Equbits Foresight
- Equbits Interpreter
- IUPAC DrawIt
- IUPAC NameIt
- KnowItAll Enterprise Server
- OptimizeIt
- PredictIt pK_a

Additional Database Options
- HaveItAll IR
- HaveItAll MS
- HaveItAll NMR
- HaveItAll Raman
- HaveItAll XNMR
- Socrates' *Infrared Characteristic Group Frequencies* CD

Additional ADME/Tox and Physicochemical Model Options

# Combine KnowItAll with the Power of Sadtler Spectra

By combining Sadtler Spectral Databases with the award-winning KnowItAll software, Bio-Rad offers a complete, unified solution for spectroscopy that is unparalleled.

Bio-Rad is the leading producer and publisher of fully verified spectral databases, with a collection that contains over 885,000 IR, NMR, MS, and Raman spectra covering pure compounds and a broad range of commercial products.

KnowItAll users can subscribe to Bio-Rad's HaveItAll® NMR, XNMR, MS, IR, and Raman database solutions. 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
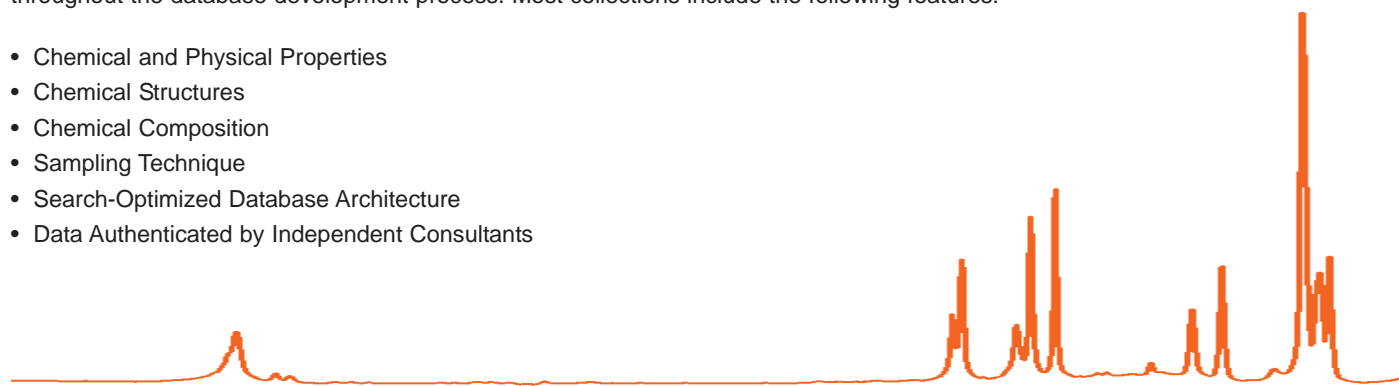
Taking KnowItAll Enterprisewide

Since the introduction of version 1.0 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 new 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 details describing the Enterprise Server and discover the advantages of elevating KnowItAll to the next level…the enterprise level.

Award-Winning KnowItAll Solutions

KnowItAll® - A Recognized Product Leader

Sadtler data solutions date back to 1874, marking over 130 years of scientific excellence. Bio-Rad's Sadtler Software & Database Solutions for Spectroscopy have been recognized as industry standards in both commercial and academic laboratories worldwide with a unique blend of spectral data, along with state-of-the-art database building, management, search, analysis, and reporting tools.

Continuing the tradition of excellence, the KnowItAll Informatics System has received many prestigious awards since its launch in 2001.

Scientific Computing & Instrumentation
Top Product of 2005 Award
(Spectroscopy Software)

Scientific Computing & Instrumentation
Top Product of 2004 Award
(Data Management – ADME/Tox)

Scientific Computing & Instrumentation
Readers' Choice Award, Finalist 2005
(Spectroscopy Software)

Scientific Computing & Instrumentation
Readers' Choice Award in 2001, 2002, 2003, and 2004
(Best Spectroscopy Software)

R&D Magazine's R&D 100 Award in 2005
(KnowItAll Multi-Technique Spectral Searching)

R&D Magazine's R&D 100 Award in 2004
(KnowItAll ADME/Tox Edition)

Frost & Sullivan's 2005
ADME/Tox Product Innovation Award, Europe

Frost & Sullivan's 2005 Drug Discovery Technologies
Market Leadership of the Year Award

Frost & Sullivan's 2003
ADME/Tox Product Differentiation Innovation Award