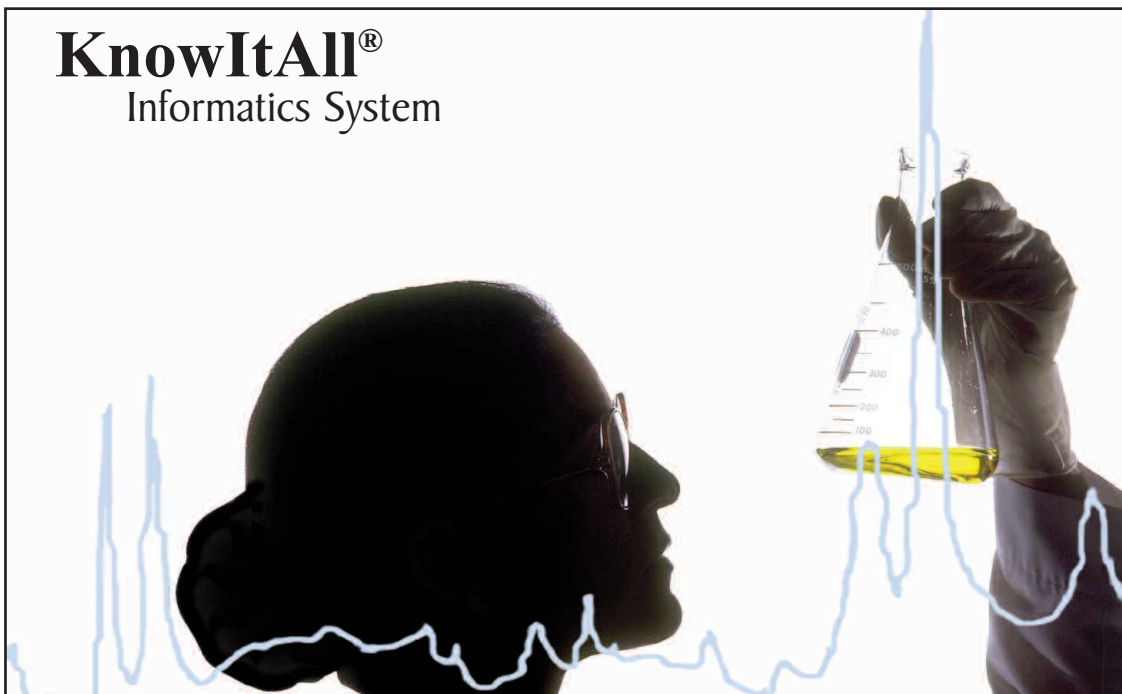
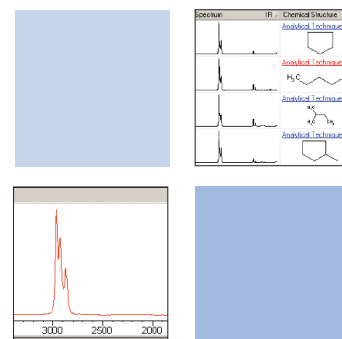


KnowItAll®
Informatics System



IR/NIR Edition



BIO-RAD

Integrated Software Solution for IR & NIR

A Truly Unique Architecture for IR/NIR Spectroscopy

The award-winning KnowItAll Informatics System, IR/NIR Edition offers the first, fully integrated software environment for infrared and Near IR. So now, researchers can finally have all the data and software solutions that they need in one place with:

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

Versatile Toolboxes.

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

True Integration.

Instantly transfer data from one application to another.

Integrated Informatics.

Manage and communicate spectroscopic, chemical, and analytical information.

The screenshot displays the MinelIt software interface. The main window shows an IR spectrum for 'LL #2 PENTANE' with a prominent peak at approximately 2900 cm⁻¹. Below the spectrum is a table of search results:

ID	Name	Spectrum	Chemical Structure
1	CYCLOPENTANE	[Spectrum]	[Structure]
2	PENTANE	[Spectrum]	<chem>CCCCC</chem>
3	2-METHYLBUTANE	[Spectrum]	[Structure]
4	METHYLCYCLOPENTANE	[Spectrum]	[Structure]
5	CYCLOHEXANE	[Spectrum]	[Structure]

On the right side, the 'Structure/Properties' panel shows the chemical structure of pentane and a table of its properties:

Name	Value	Unit
Name	PENTANE	
Source of Sample	ALDRICH CHEMICAL COMPANY, INC., MILWAUKEE, WISCONSIN	
Technique	NEAT	
Melting Point	-129.72C	
Boiling Point	36.07C	
Density	20C=0.62624; 25C=0.62139 G/ML	
Flash Point	-40F	
Mol.Weight	72.15	
Optical Properties	Index of Refraction= 20C=1.35748; 25C=1.35472	
Dielectric Constant	1.844 (20C)	
CAS Registry Number	109-66-0	
Formula	C5H12	
Vapor Pressure	512.5 TORR	
Comments	VOLATILE LIQUID, SLIGHTLY SOLUBLE	

At the bottom right, there is a 'Desktop & Enterprise Solutions.' logo.



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

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.

What is in this Edition?

The KnowItAll IR/NIR Edition offers the following applications and options. Full details on each application is outlined in this brochure.

Data Toolbox

SearchIt™	Database searching (full spectrum, structure, peak, property, etc.)
Minelt™	Database display and mining
Database Building (optional)	Build databases with IR/NIR spectra and structures; feature in Minelt
Overlap Density Heatmap	Patented technology for visual datamining and analysis; feature in Minelt
Pirouette® Model Support	Use models built in Infometrix' Pirouette software
Batch Property Calculation	Calculate properties for entire database
CompareIt™	Data plotting and visualization
Mixture Analysis	Analyze experimental spectral data of mixtures

Spectral Analysis Toolbox

AnalyzeIt™ IR (optional)	IR spectrum/structure correlation
ValidateIt™	Statistical model validation
AnalyzeIt™ MVP (optional)	Multivariate processing
AnalyzeIt™ Polymer IR (optional)	IR spectrum/structure correlation for polymeric compounds

Spectral Processing Toolbox

Refinelt™ IR	IR spectrum processing
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Basics Toolbox

DrawIt™	2D structure drawing (includes stereochemical recognition)
ReportIt™	Publish professional reports, with structures, spectra, and more
BrowseIt™	Portal for KnowItAll users with useful links to technical information, etc.

Optional Solutions

In addition to the tools and options above, here are some other solutions available to you with the KnowItAll IR/NIR Edition:

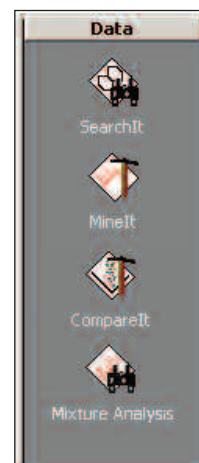
Infometrix Pirouette Software	Additional chemometrics tools for classification, data exploration, and multivariate regression
IUPAC DrawIt™	IUPAC name to structure
IUPAC NameIt™	Structure to systematic IUPAC name
KnowItAll® Enterprise Server	Centralize spectral and chemical information on the KnowItAll server
Socrates IR CD	Resource for functional group analysis
Upgrade Plan	Support and upgrade plan for KnowItAll users

Optional Spectral Databases

HaveItAll® IR IR & NIR Databases	Annual license to over 220,000 IR spectra Choose from over 100 spectral databases
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Data Toolbox

With the Data Toolbox, researchers can build, search, and mine user-generated or reference databases containing analytical (including spectra), chemical, and additional metadata.



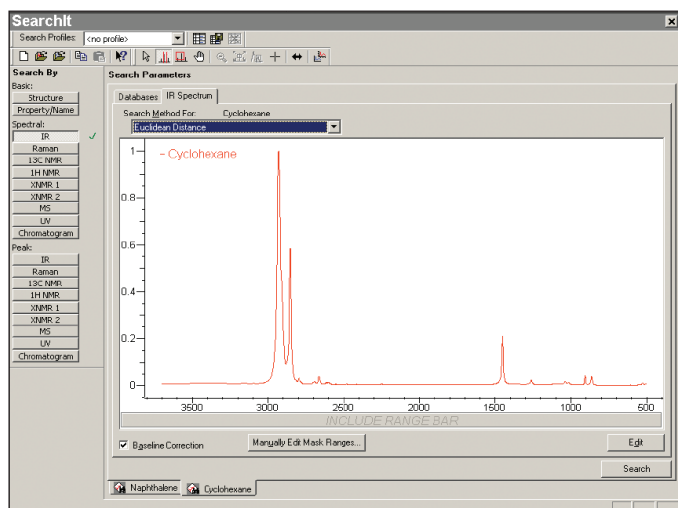
SearchIt™

Database Searching

The SearchIt application allows researchers to import their 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 IR and NIR spectra)—in any combination.

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.



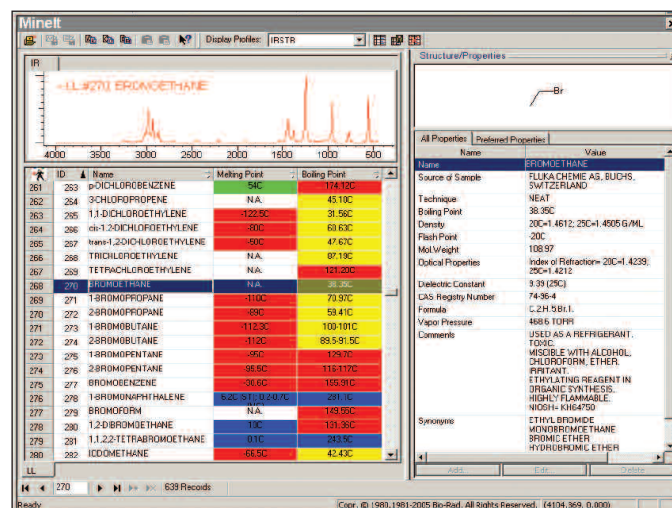
MineIt™

Database Viewing & Mining

MineIt is a deceptively simple application. Like Microsoft Word, it is easy for beginners, but has many advanced features that more sophisticated users will appreciate. With MineIt, users can view reference databases, user-created databases, or hit lists generated by the companion SearchIt application.

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.



Database Building

(Optional Feature in the Minelt Application)

Build Searchable Databases with Spectra, Structures, & Properties

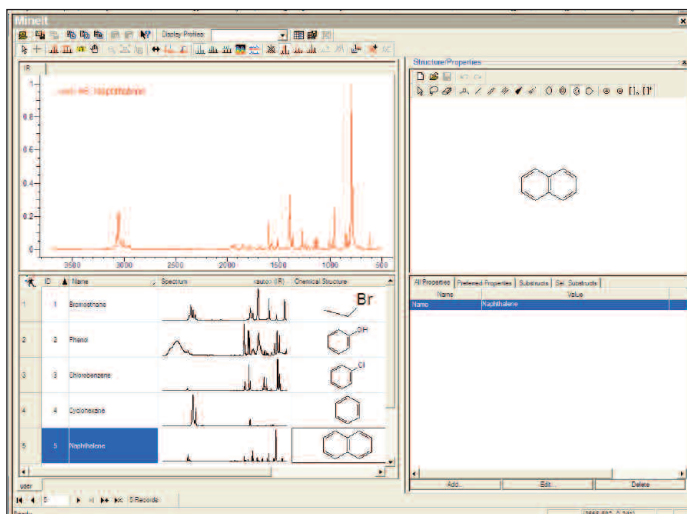
Chemists and spectroscopists produce valuable data every day within their organizations. When Minelt is combined with the power of the Database Building Option, researchers can capture these resources and build searchable databases that include IR and NIR spectra, chemical structures, and alphanumeric data. And with KnowItAll, you have the option to deploy data management at the desktop or enterprise-wide.

Import Experimental Data Even if Laboratory has Instruments from Multiple Vendors

Analytical spectra can be imported in native format for many common instrument makes and models or in *.csv format (spreadsheet or textfile). So even if a laboratory's analytical instruments come from multiple manufacturers, KnowItAll can archive the data.

Researchers can also import multiple structure formats with stereochemical bonds and identifiers. Users can easily import structures in MOL and SDF file formats to create databases quickly from existing data.

The software also offers a batch import and export capabilities for handling of spectra, structures, and property files.



Customize & Protect Databases

Databases can be customized to meet each laboratory's specifications. Archive spectral data to include peak information, structures, and properties, such as source of sample, boiling point, etc.

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.

Add Hyperlinks to Web Pages and Other Documents

Users can make databases even more powerful by linking records to web pages, spreadsheets, and other documents. After links are created, researchers can click on the hyperlink to open the document or web page.

Cross-Reference to Other Datasets*

With Minelt, users can cross-reference analytical data in one record to analytical data in another record; for example, an IR spectrum can be linked to an NIR spectrum. Once the cross-reference is created in the database, the user can click on the "Other Techniques" link and go directly to the other data available for that compound. Structure and property information can then be shared between different analytical techniques to increase productivity and avoid errors.

Supports Data Export

The KnowItAll database file format is a secure, stable, and instrument vendor-neutral platform where multi-technique spectra, chromatograms, structures, and data can be stored for long periods of time.* In addition to importing data, KnowItAll also supports exporting data, which, unlike many other spectral database systems, allows you the freedom and flexibility in the future. Other systems lock you in; KnowItAll does not.

* If you wish to include additional analytical techniques (including NMR, MS, Raman, UV-Vis, chromatography) in your databases, please ask about the KnowItAll Analytical Edition.

Overlap Density Heatmap

(Feature in the Minelt Application)

Patented 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, obliterate trends when viewing large amounts of data.

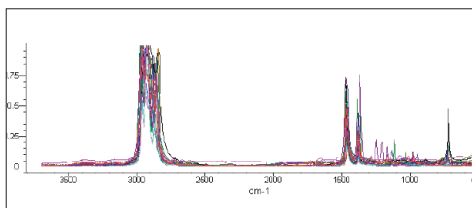
Bio-Rad is pleased to announce a new breakthrough technology for visual data mining and analysis that can now turn these unmanageable amounts of data into actionable information. Part of the KnowItAll Informatics System, Overlap Density (OD) Heatmap and OD Consensus object technologies allow trends to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

How Does It Work?

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

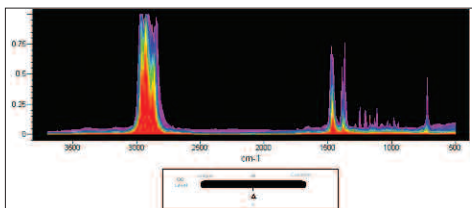
Traditional Stacked Display

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



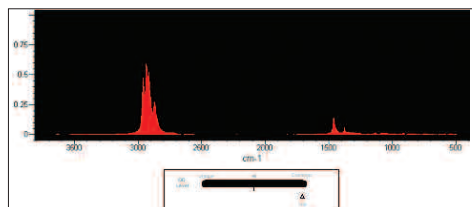
OD Heatmap OD Level = 0

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.



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.

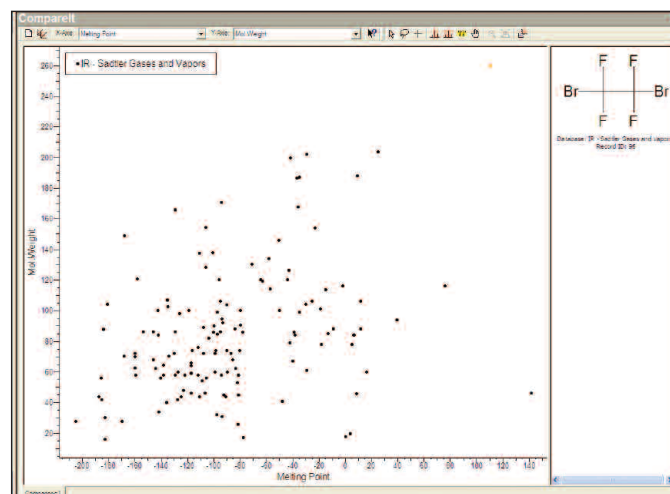
Visualizing Data Trends

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 Indices - HQIs) against each other, such as IR HQI versus NIR 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.

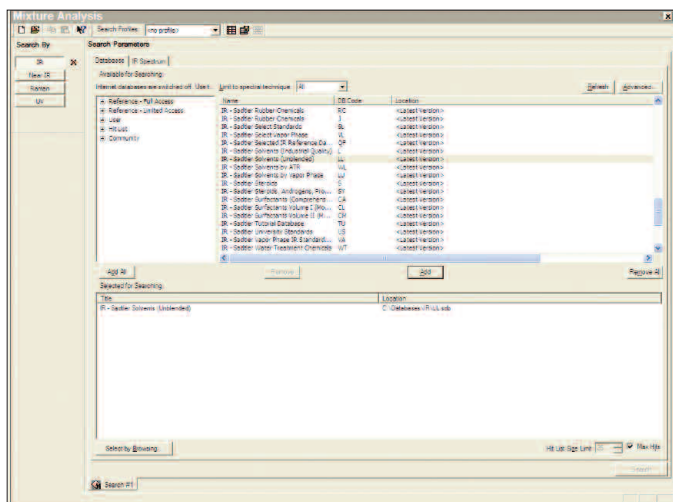




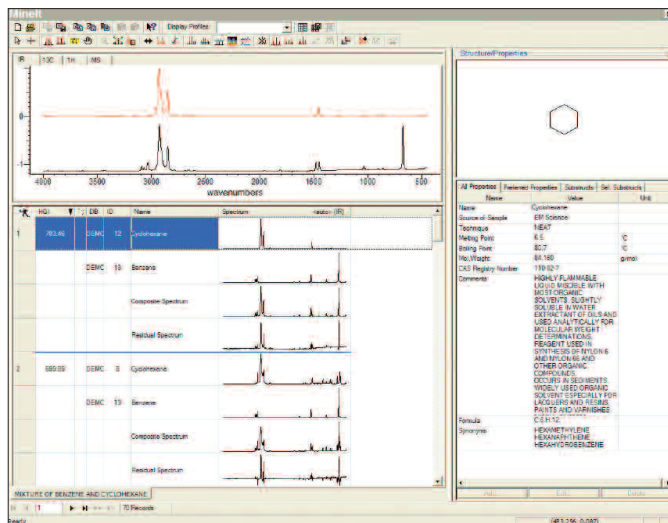
Mixture Analysis

Analyze Experimental Spectral Data of Mixtures

This application deconvolutes components of a mixture by analyzing a spectrum. It allows comparison 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.



Analyzelt™ MVP (Optional Application)

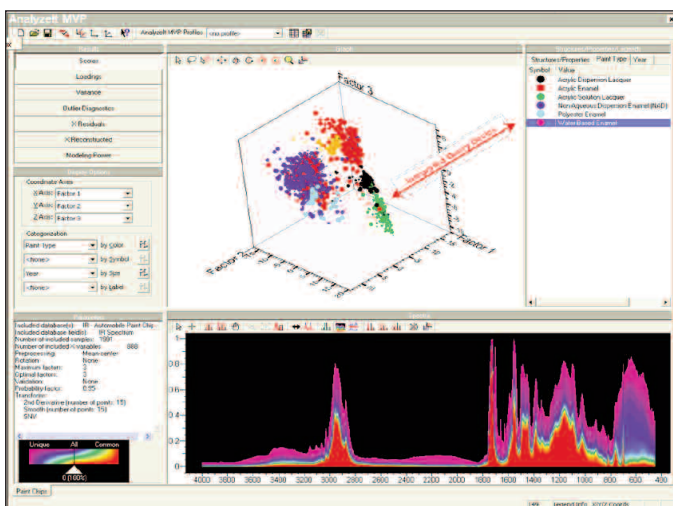
Multivariate Processing Made Simple

The elegance and power of Infometrix Pirouette chemometrics software are a perfect complement to the cheminformatics and comparative visualization tools in the KnowItAll system. The result is an advanced tool for multivariate processing to analyze spectroscopic 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.



Analyzelt™ Polymer IR (Optional Application)

Interpret the IR Spectra of Polymer Compounds.

KnowItAll's Analyzelt Polymer IR is an application developed to aid in the interpretation of the bands in an infrared spectrum specifically for polymeric compounds.

How Does it Work?

Simply load a spectrum and click on a peak of interest to compare to the Analyzelt Polymer IR knowledgebase to generate a list of all functional groups possible at that position. You can also view each structural fragment, along with other regions where these fragments would contain peaks.

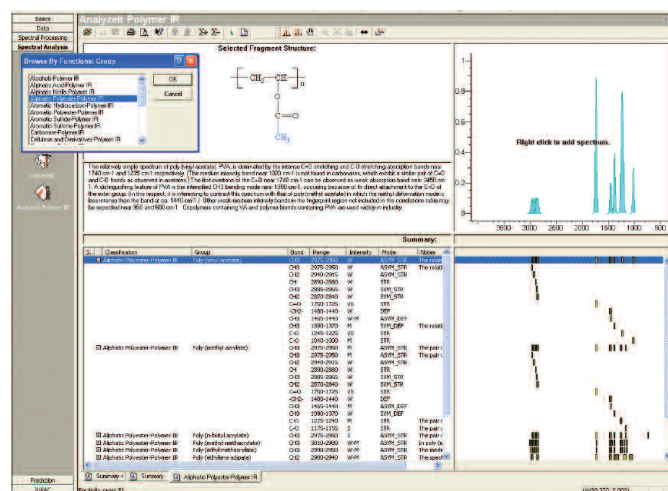
A summary of the most likely candidates (positive interpretations) is maintained to assist in narrowing the interpretation. The application even highlights the bonds involved in the vibrational frequency.

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

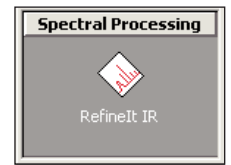
Key Features

- Knowledgebase of 100 functional groups
- Knowledgebase contains hundreds of interpretation frequencies
- Import experimental spectral data
- Intelligent "Suggest a Peak" feature
- Summarize negative or positive interpretations
- Browse knowledgebase by chemical class
- Peak overlay display
- Displays & highlights structural bonds
- View notes for functional groups when available
- Build knowledgebases of functional groups that can be used in the interpretation
- For those expert and non-expert in polymer interpretation alike



Spectral Processing Toolbox

The Spectral Processing Toolbox offers a powerful application for processing spectra.



IR Spectrum Processing

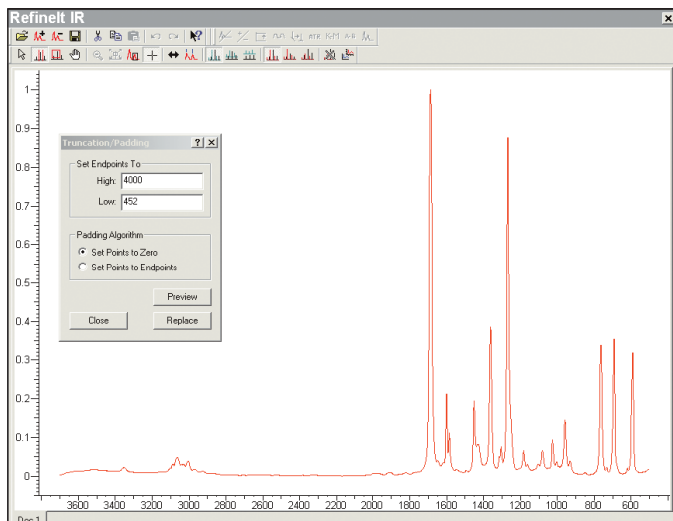
RefineIt IR provides a variety of tools to process spectra and improve both the quality of search results and the overall look of publications. RefineIt IR can also be used in conjunction with other KnowItAll applications. For example, a spectrum can be transferred from the SearchIt application to RefineIt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

Processing capabilities 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

Analytical capabilities include:

- Area Under the Curve (AUC)



Basics Toolbox

The Basics 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.



DrawIt™

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

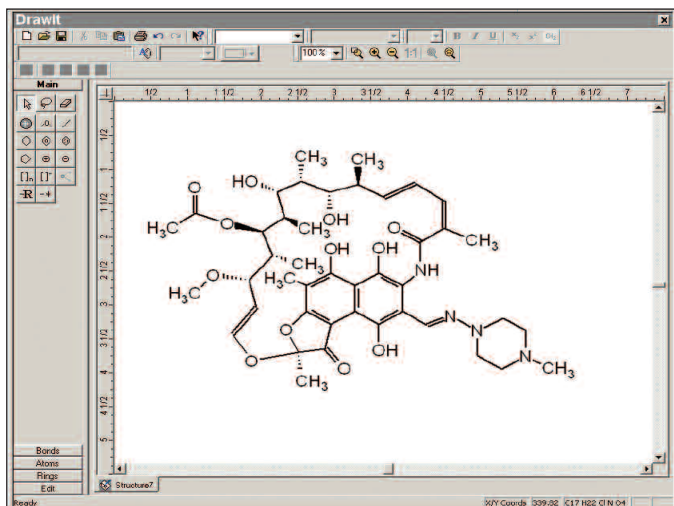
DrawIt provides an advanced set of drawing tools—just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

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** (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.



BrowseIt™

Integrated Web Resources

BrowseIt is a web browser built into the KnowItAll Informatics System, which provides access to a website designed especially for KnowItAll users. This site offers demo movies, tips, and the latest KnowItAll product information.

Basics



DrawIt



ReportIt



BrowseIt



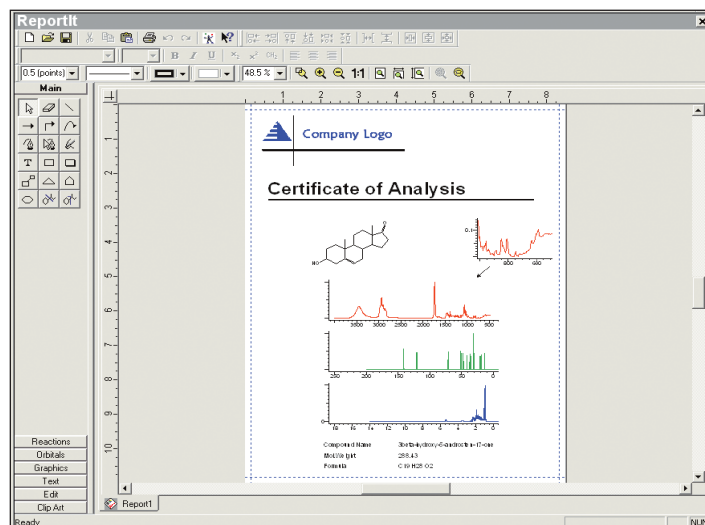
ReportIt™

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 and 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 3D drawings
- **Table Tool** to enter and organize data
- **Spectrum 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, including axes, colors, labels, etc.
- **Custom Annotation Tool** to link objects like spectral peaks to text graphics or chemical structure captions



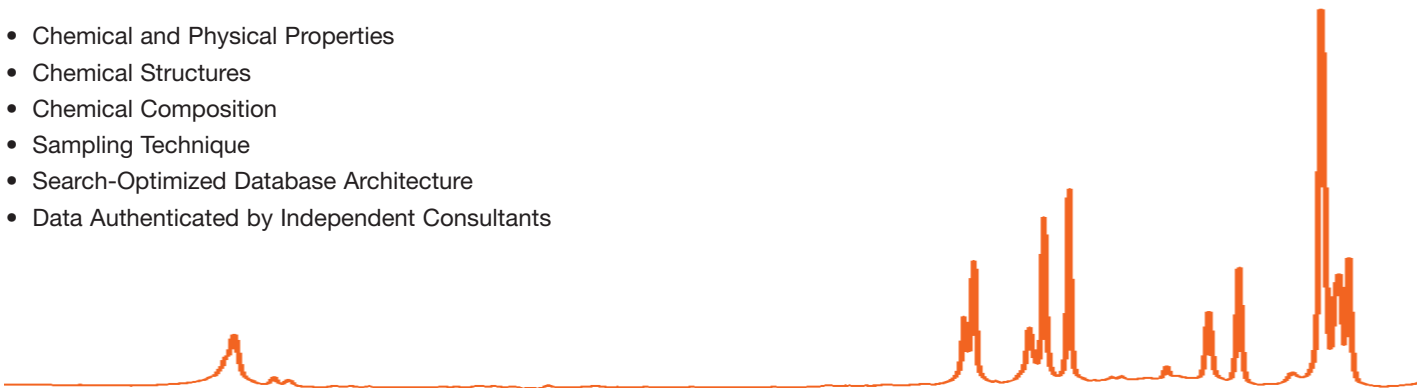
Spectral Databases with KnowItAll

Bio-Rad is the leading producer and publisher of fully verified spectral databases, with a collection that contains over 1.3 million IR, NMR, MS, Raman, NIR, 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 its 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 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 organization—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.

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
Readers' Choice Silver & Gold Awards in 2008
(Best Spectroscopy & Chemistry Software)



Scientific Computing
Readers' Choice Silver Award in 2007
(Best Spectroscopy Software)



Scientific Computing
Readers' Choice Silver & Gold Awards in 2006
(Best Spectroscopy & Cheminformatics Software)



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



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

Scientific Computing
Top Product of 2005 Award
(Spectroscopy Software)



Scientific Computing
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

www.knowitall.com

Minimum System Recommendations: Requires the KnowItAll Informatics System. For a current list of minimum system requirements including operating system, processor, RAM, disk space, please visit www.knowitall.com/system_recommendations

BIO-RAD

**Bio-Rad
Laboratories**

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