Software for IR, NIR, & Raman

KnowItAll® Vibrational Spectroscopy Edition

BIO-RAD

Overview

Bio-Rad's award-winning **KnowItAll Informatics System** - **Vibrational Spectroscopy Edition** offers comprehensive software solutions for infrared, near infrared, and Raman spectroscopy in a single, integrated interface.

The software package includes all the following tools:

- Spectral Search
- Spectral Identification
- IR Spectral Deformulation
- Mixture Analysis
- Functional Group Analysis - IR, Raman, IR Polymer
- Over 12,000 IR Spectra
- Spectral Data Management (Database Building)
- Processing & Subtraction
- Quality Control Analysis
- Chemical Structure Drawing - ChemWindow®
- Reporting Tools
- Training Resources
- Patented Ovelap Density Heatmap Technology for Data Visualization
- Patent-Pending Optimized Corrections Technology to Optimize Spectral Searchs

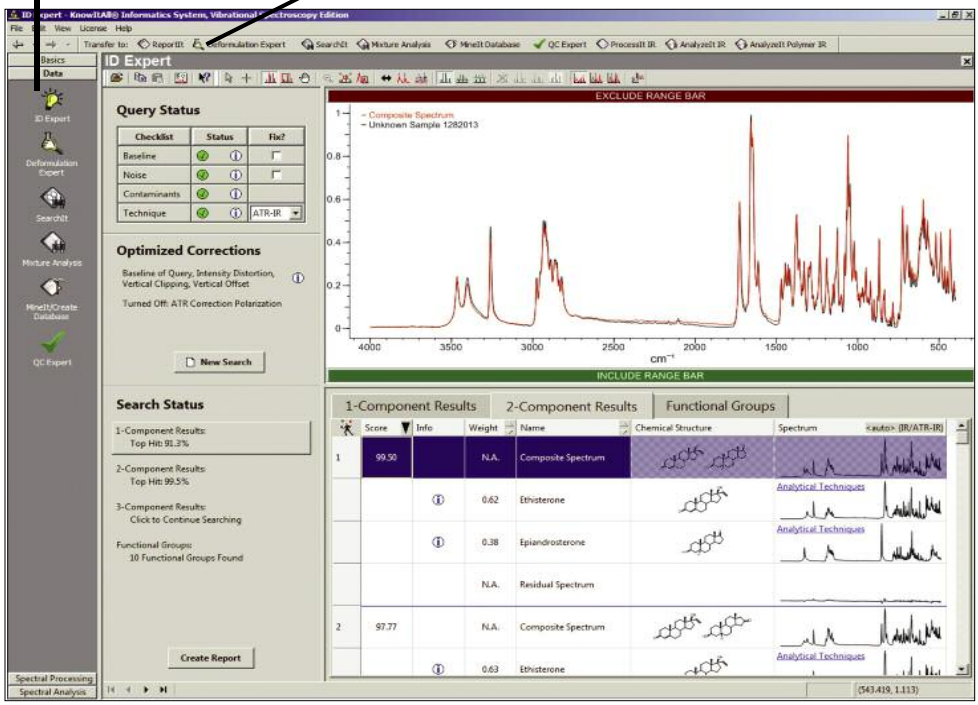
Includes cutting-edge technologies only available from Bio-Rad, as spectral intelligence is continually added to the KnowItAll software, helping chemists find the best answers and extract the most knowledge from spectral data.

Supports file formats from all major IR, NIR, and Raman spectrometer instrument vendors.

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.



What Is Included?

The KnowItAll Vibrational Spectroscopy Edition includes the following tools and options.

Data Toolbox

ID Expert™	Spectral identification software with built-in spectral intelligence
Deformulation Expert™	Reverse engineering of IR spectra of commercial products into pure components (Requires a subscription to the KnowItAll IR Spectral Library to view unlocked results)
SearchIt™	Database searching (full spectrum, structure, peak, property, etc.)
MineIt™/Database Building	Build multi-technique databases with spectra and structures; data display and mining
Mixture Analysis	Analyze experimental spectral data of mixtures
QC Expert™	Perform a quality check of sample IR or Raman spectrum against a reference spectrum

Spectral Analysis Toolbox

AnalyzeIt™ IR	IR functional group analysis
AnalyzeIt™ Raman	Raman functional group analysis
AnalyzeIt™ Polymer IR	IR spectral interpretation for polymeric compounds
AnalyzeIt™ MVP *(optional)*	Multivariate processing for chemometrics
ValidateIt™	Model validation

Spectral Processing Toolbox

ProcessIt™ IR	IR spectrum processing
ProcessIt™ Raman	Raman spectrum processing

Basics Toolbox

ChemWindow®	2D structure drawing
ReportIt™	Publish professional reports, with structures, spectra, and more
BrowseIt™	Web portal with links to training information

Spectral Databases

Over 12,000 IR Spectra	This package includes several databases

Optional Solutions

KnowItAll IR Spectral Library	Worlds largest database of IR spectra
KnowItAll Raman Spectral Library	Fastest-growing database of high-quality Raman spectra
Infometrix Pirouette Software	Additional chemometrics tools for classification, data exploration, and multivariate regression
KnowItAll® Enterprise Server	Centralize spectral and chemical information on the KnowItAll server
Upgrade Plan	Support and upgrade plan for KnowItAll users

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

Data Toolbox

ID Expert™

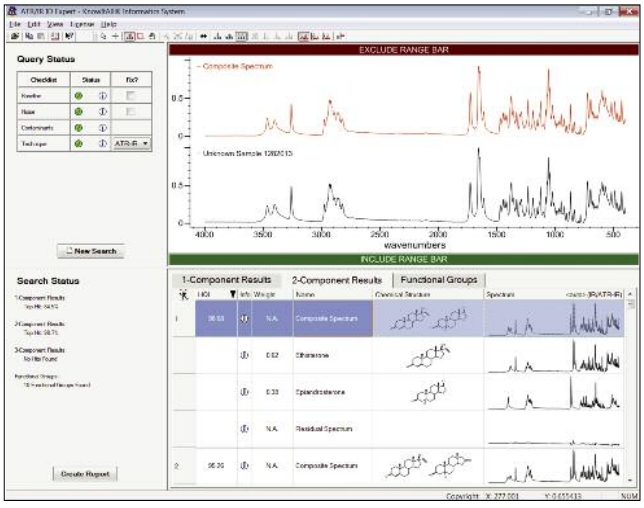
Infrared & Raman Spectral Identification

KnowItAll® ID Expert™ is a completely new technology that combines Bio-Rad's years of accumulated knowledge with tremendous software processing power to provide the fastest, most accurate answer possible to scientists identifying unknown IR & Raman spectra.

Simply open an unknown spectrum and ID Expert automatically performs single component searches, multiple component searches, peak searches, and functional group analyses simultaneously and summarizes the results on a single screen to give a complete view of all possibilities for the unknown spectrum.

If there are problems with the user's query spectrum, ID Expert has the spectral intelligence to identify these issues and suggest ways to fix them.

The spectral intelligence built into KnowItAll ID Expert—when used with Bio-Rad's KnowItAll IR and Raman Spectral Libraries—provides the highest level of expertise to any scientist, whether a novice or power user.



Deformulation Expert™

Reverse Engineer Commercial Products of IR Spectra

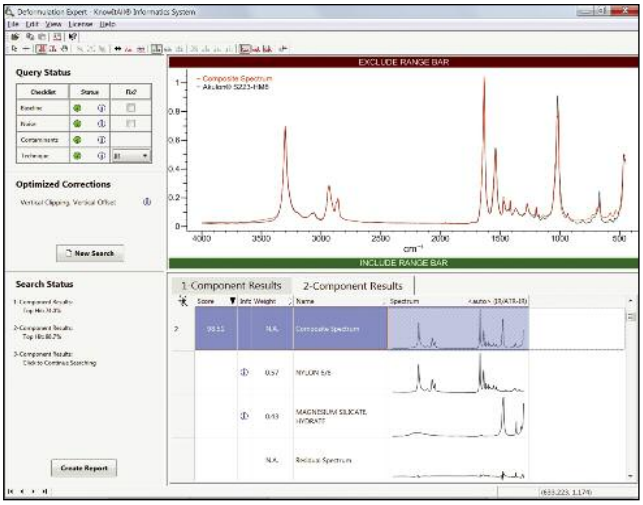
KnowItAll Deformulation Expert assists scientists with:

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

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

If there are problems with the user's query spectrum, Deformulation Expert has the spectral intelligence to identify these issues and suggest ways to fix them.

Deformulation Expert requires a subscription to the IR KnowItAll Spectral Library to view unlocked results.



SearchIt™

Database Searching

SearchIt allows researchers 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, spectra, and peak—in any combination.

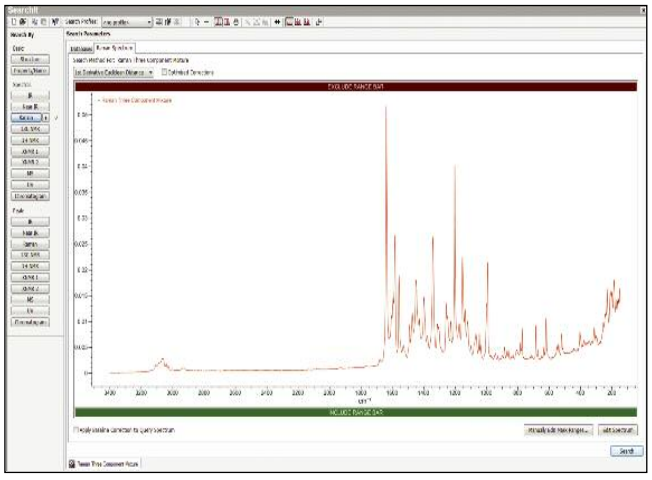
Advanced Spectral Searching

SearchIt permits both full spectrum searching, as well as 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.

New Technology to Find Optimal Spectral Matches in Reference Databases

Bio-Rad's Optimized Corrections a patent-pending technology that performs a computationally complex set of corrections on all query and reference spectra in a search to find the optimal match between the query and each reference spectrum. Multiple corrections are applied automatically to compensate for differences between spectra caused by the variability of different instruments and accessories as well as other factors, including human error.

Corrections include: baseline correction, clipping, horizontal shift, vertical shift, intensity distortion, and ATR correction (if needed).

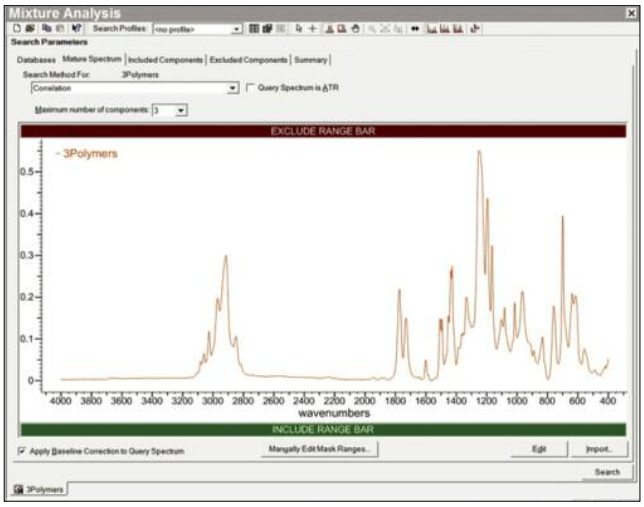


Mixture Analysis

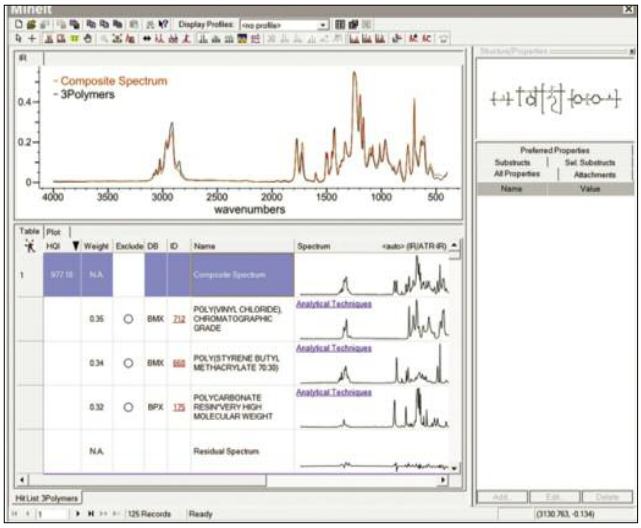
Analyze Experimental Spectral Data of Mixtures

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.



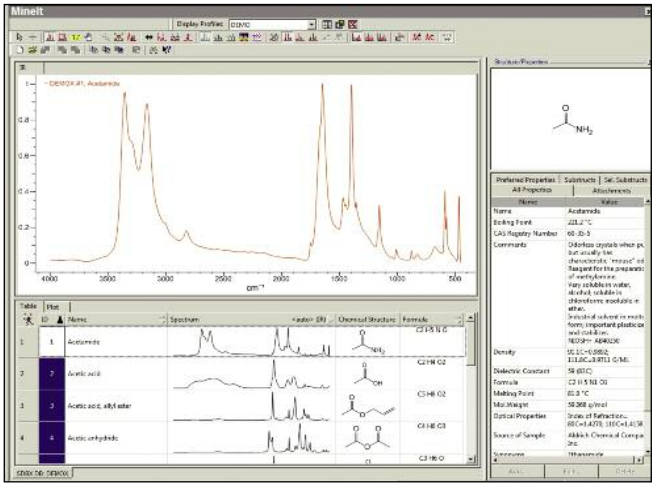
Results show possible components in the mixture.

MineIt™ Database Building

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, the KnowItAll solutions have been built through years of experience in doing just that—building databases.

Researchers can build searchable databases that include one or more vibrational spectroscopy techniques (IR, Raman, Near IR), chemical structures, and other metadata. So even if a laboratory's analytical instruments come from multiple manufacturers, KnowItAll can archive the data.



Key Features

Centrally Store & Share Spectral Data

- Build databases with one or more techniques (IR, NIR, Raman)
- 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
- "Auto-Property" computes values such as formula, molecular weight, etc. on entire datasets
- Make database more powerful by attaching spreadsheets, MSDS, and other documents or adding hyperlinks to web pages
- Create cross-reference from record to data from another technique; i.e., a Raman spectrum can be linked to an IR spectrum
- 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
- Quickly add properties & structures from PubChem to your database.

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

Database Mining & Visualization

Database Viewing & Mining

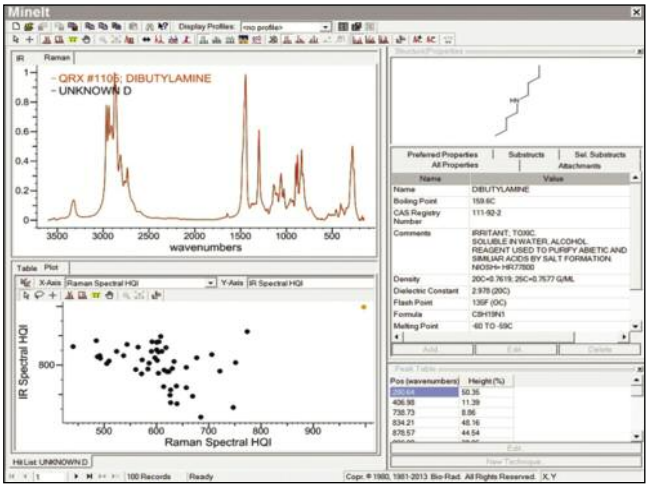
With MineIt, users can view reference databases, user-created databases, or search results.

Access Data from Multiple Techniques

The unified KnowItAll environment includes a powerful feature that allows the user to access databases containing IR, Raman, and NIR spectra; 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).

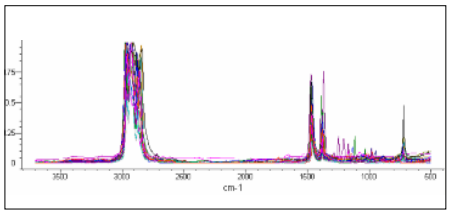
Overlap Density Heatmaps: Patented Technology for Visual Data Mining & Analysis

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.

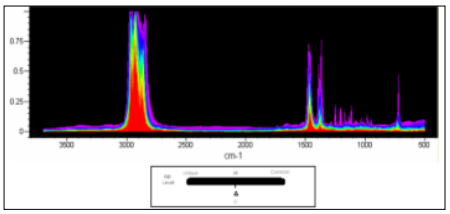
Traditional Stacked Display

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



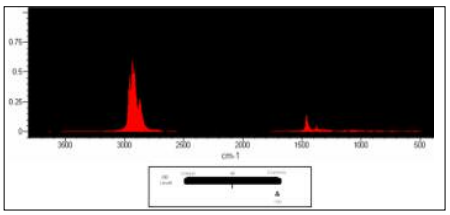
OD Heatmap OD Level = 0

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

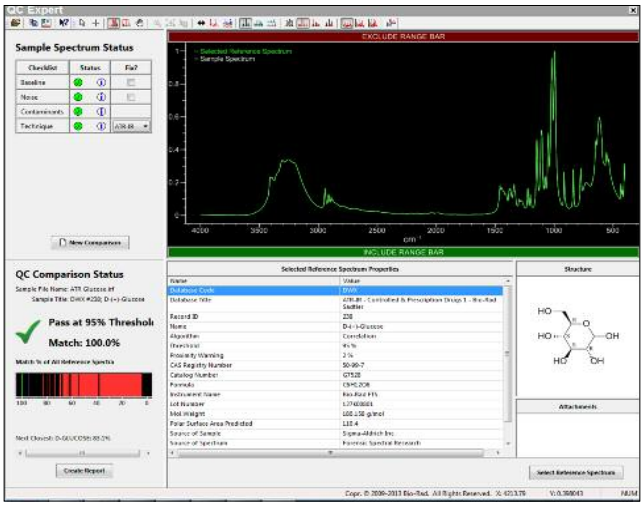
An Overlap Density Heatmap showing only those areas of overlap common to all spectra.



QC Expert™

IR & Raman Quality Control Comparison

Bio-Rad's KnowItAll QC Expert software performs a rapid quality check of a sample IR or Raman spectrum against a "gold standard" user spectrum to verify that a material meets control specifications.



Key Features

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

Spectral Analysis Toolbox

AnalyzeIt™ IR & Raman

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

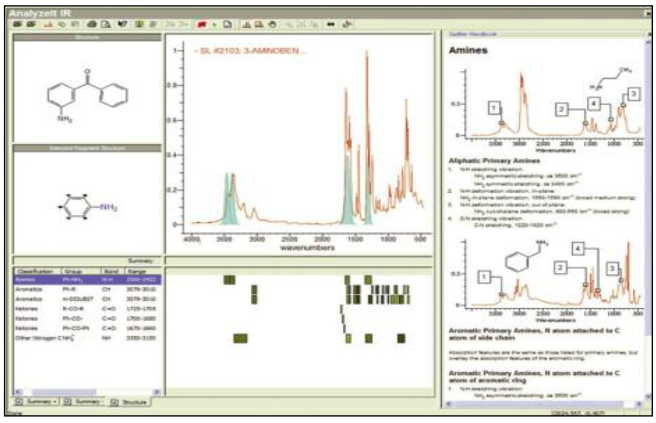
Improve spectral interpretations by building knowledgebases of functional groups to use with AnalyzeIt’s knowledgebase.

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 and/or positive interpretations
- Peak overlay display for easy comparison
- Display/highlight bonds involved in vibrational frequency
- Build your own knowledgebase to use in analyses
- For those expert and non-expert in spectral interpretation alike
- Link to additional data in Sadtler Handbook (AnalyzeIt IR only)



AnalyzeIt™ Polymer IR

Interpret IR Spectra of Polymers

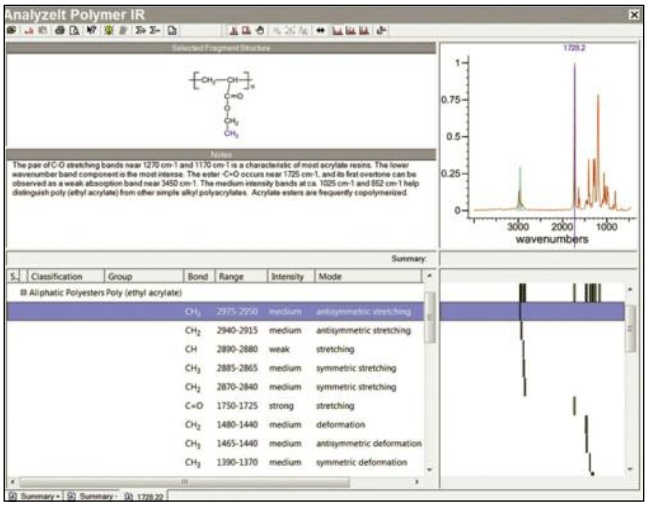
Simply load a spectrum and click a peak of interest; AnalyzeIt then lists all functional groups possible at that peak position. Compare peak regions for each group by overlaying with the spectrum and narrow results by tagging the “most likely” candidates.

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 & 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



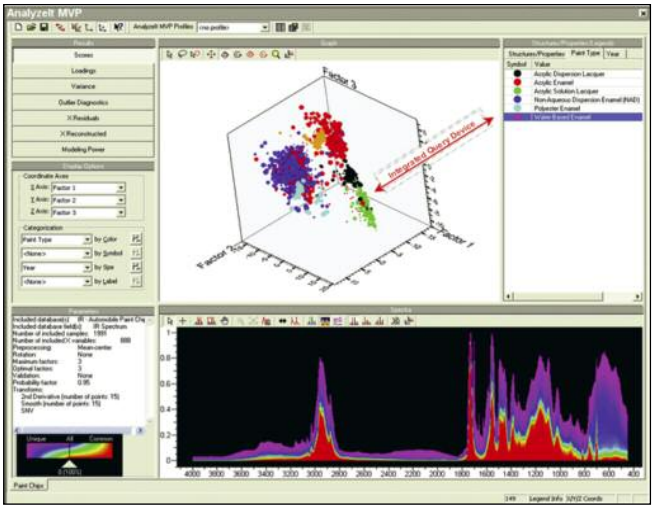
AnalyzeIt™ MVP *(Optional)*

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, 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, or investigation



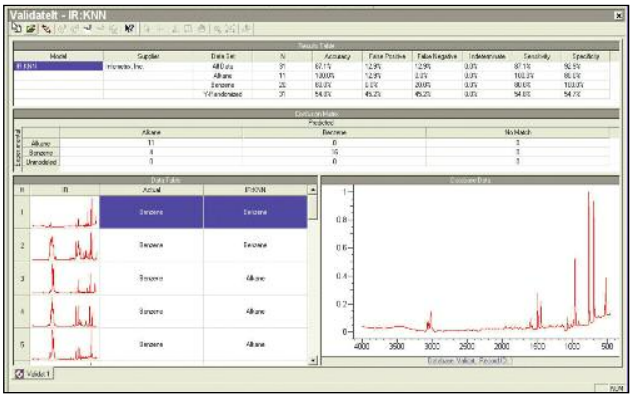
What is Multivariate Analysis? *Multivariate analysis (including principal component analysis, PCA) refers to the statistical analysis techniques where multiple variables are analyzed to determine the contribution made by each variable to an observed result. This permits patterns to emerge from within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

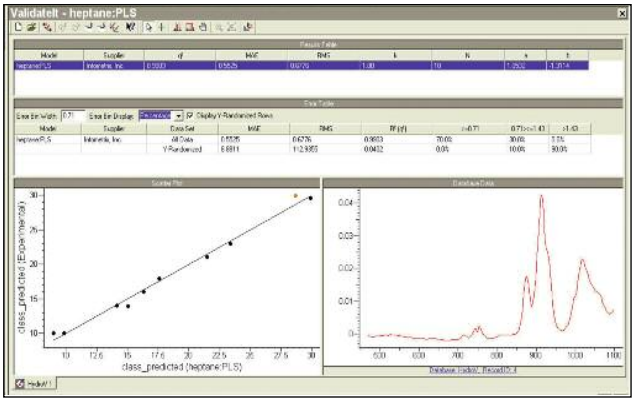
ValidateIt™

Predict & Validate by Spectrum

The ValidateIt tool allows a user to test a Pirouette 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.





Spectral Processing Toolbox

ProcessIt™ IR

IR Spectrum Processing

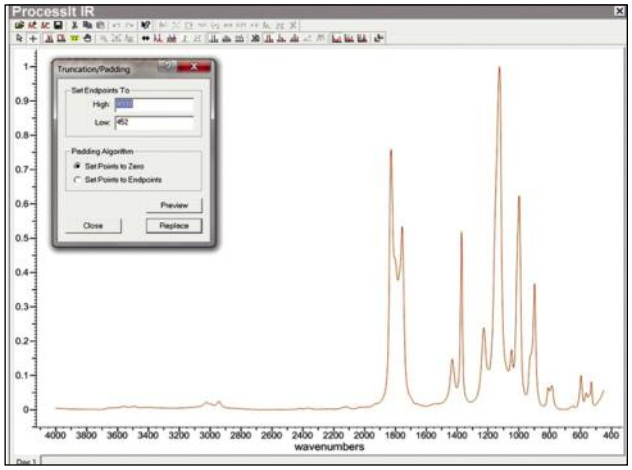
ProcessIt IR provides a variety of tools to process spectra and improve the quality of archived data and search results. ProcessIt IR can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to ProcessIt IR to correct potential searching problems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

Analytical Capabilities Include:

- Area Under the Curve (AUC)



ProcessIt™ Raman

Raman Spectrum Processing

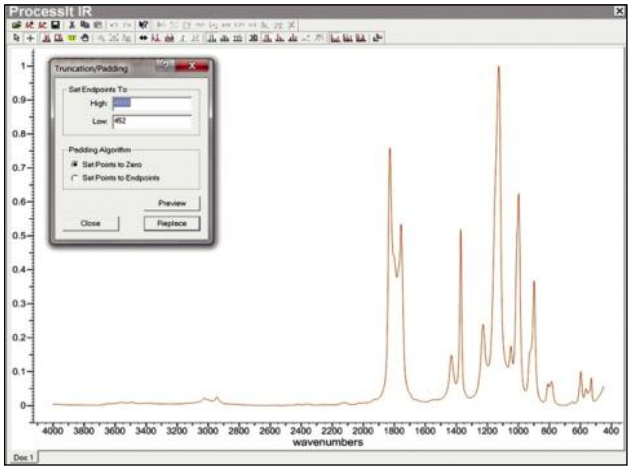
ProcessIt Raman provides a variety of tools to process spectra and improve the quality of archived data and search results. ProcessIt Raman can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to ProcessIt Raman to correct potential searching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

Processing Capabilities Include:

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

Analytical Capabilities Include:

- Area Under the Curve (AUC)



Basics Toolbox

ChemWindow®

A Full-Featured 2D Structure Drawing Program

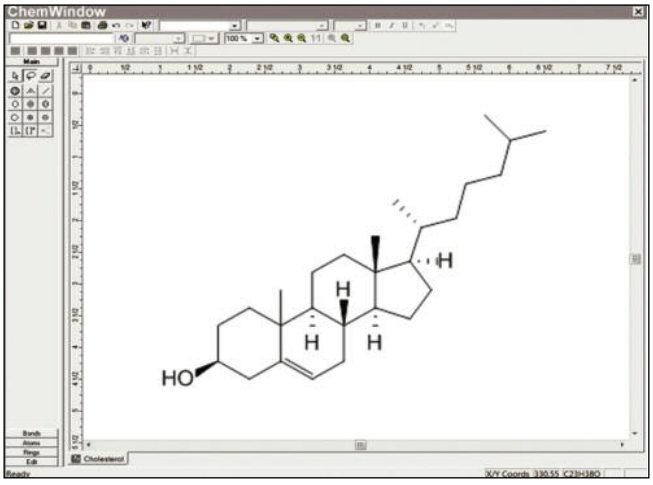
ChemWindow® provides an advanced set of drawing tools—just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

Key Features:

- Customizable toolbars with tools to draw chemical structures, including bonds, rings, atom labels, charges, etc.
- Chemical recognition features such as hot keys, chemical syntax checker, tools to calculate mass and formula, etc.
- 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 ChemWindow. MOL files can also be imported. Many other file formats are also supported.



BrowseIt™

Web Training Resources

BrowseIt is a web browser built into the KnowItAll software with links to KnowItAll tutorial movies and a discussion board for KnowItAll users.

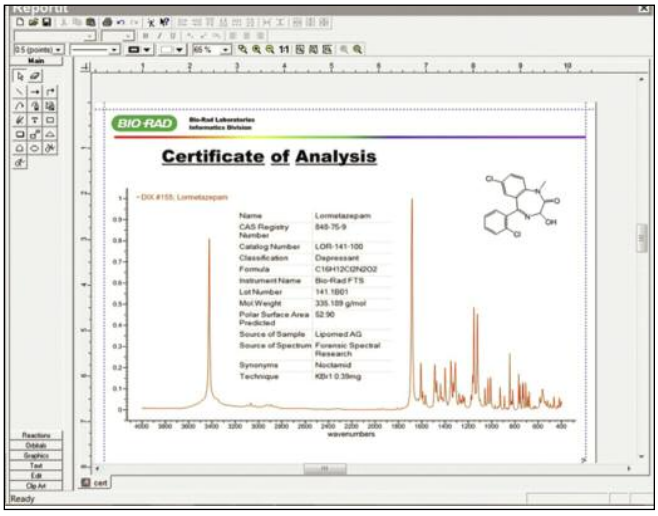
ReportIt™

A Full-Featured Publishing Program

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

Key Features:

- Custom templates to create uniform reports for enterprise-wide format standardization
- Customizable toolbars to draw chemical reactions and other reports, including arrows, text boxes, shapes, etc.
- Clip art libraries with hundreds of laboratory glassware drawings and engineering symbols
- OLE technology (Object Linking and Embedding) for in-place editing in word processing and presentation software
- MS fragmentation tool to display a mass for each fragment
- Advanced editing options to align, space, center graphics, and rotate captions
- Predefined styles for captions and structures
- 3D structure visualization for high-quality, realistic 3D drawings
- Table tool to enter and organize 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.
- Annotation tool to link objects like spectral peaks to text graphics or chemical structure captions



Includes Over 12,000 IR Spectra

The KnowItAll Vibrational Spectroscopy Edition includes the following databases:

- IR - Standards (Organic & Polymeric Compounds Subset) - Bio-Rad Sadtler - 9,996 spectra
- IR - Polymers, Hummel - Bio-Rad Sadtler - 1,907 spectra
- ATR-IR - Solvents - Bio-Rad Sadtler - 629 spectra

Bio-Rad also offers subscriptions to its complete libraries of IR and Raman spectra. Please contact us for more information.

www.knowitall.com

BIO-RAD

Bio-Rad
Laboratories, Inc.

For System Recommendations visit **http://www.knowitall.com/system_recommendations**

Informatics Division **Website:** www.knowitall.com **Contact Us:** www.knowitall.com/contactus

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