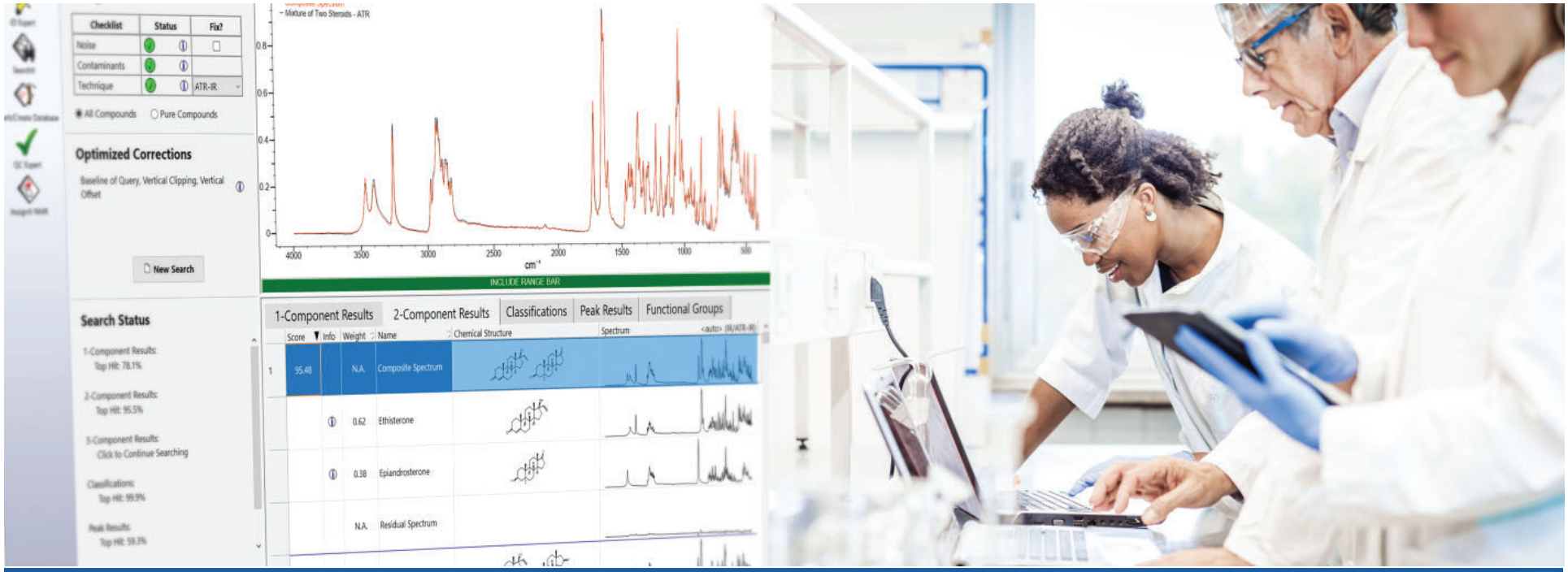
From the Leader in Spectral Databases



KnowItAll Spectroscopy Edition

Software Solutions for IR, MS, NMR, Raman, & UV-Vis

Available in English, Japanese, Chinese, French, and German

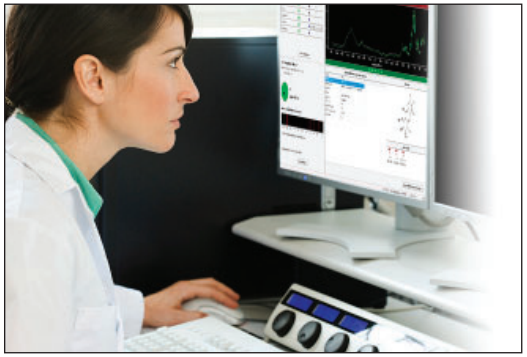
WILEY

Whether you use one or more techniques, KnowItAll spectroscopy software has the right solution for your lab!

Wiley's **KnowItAll Spectroscopy Edition** offers solutions to identify, analyze, and manage spectral data. It supports multiple instrument vendor file formats and techniques, including **IR, MS, NMR, Raman, and UV-Vis**.

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

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



Accessibility features like keyboard access to menus, audio narration for icons, and tool tips.

**Subscription required to the KnowItAll Libraries*
KnowItAll and ChemWindow are trademarks of Wiley in certain jurisdictions.

Key Features

- Basic Spectrum Analysis
- Advanced Spectrum / Mixture Analysis
- Name and Property Search
- Database Building / Management
- Structure Drawing / Reports (ChemWindow)
- Spectrum Processing
- Comprehensive KnowItAll IR, MS, NMR, Raman, UV-Vis library subscriptions available*
- Technique-specific tools: 12K bonus IR spectra, functional group analysis, MS reverse & adaptive search (patent pending), NMR prediction & more!

Data Types

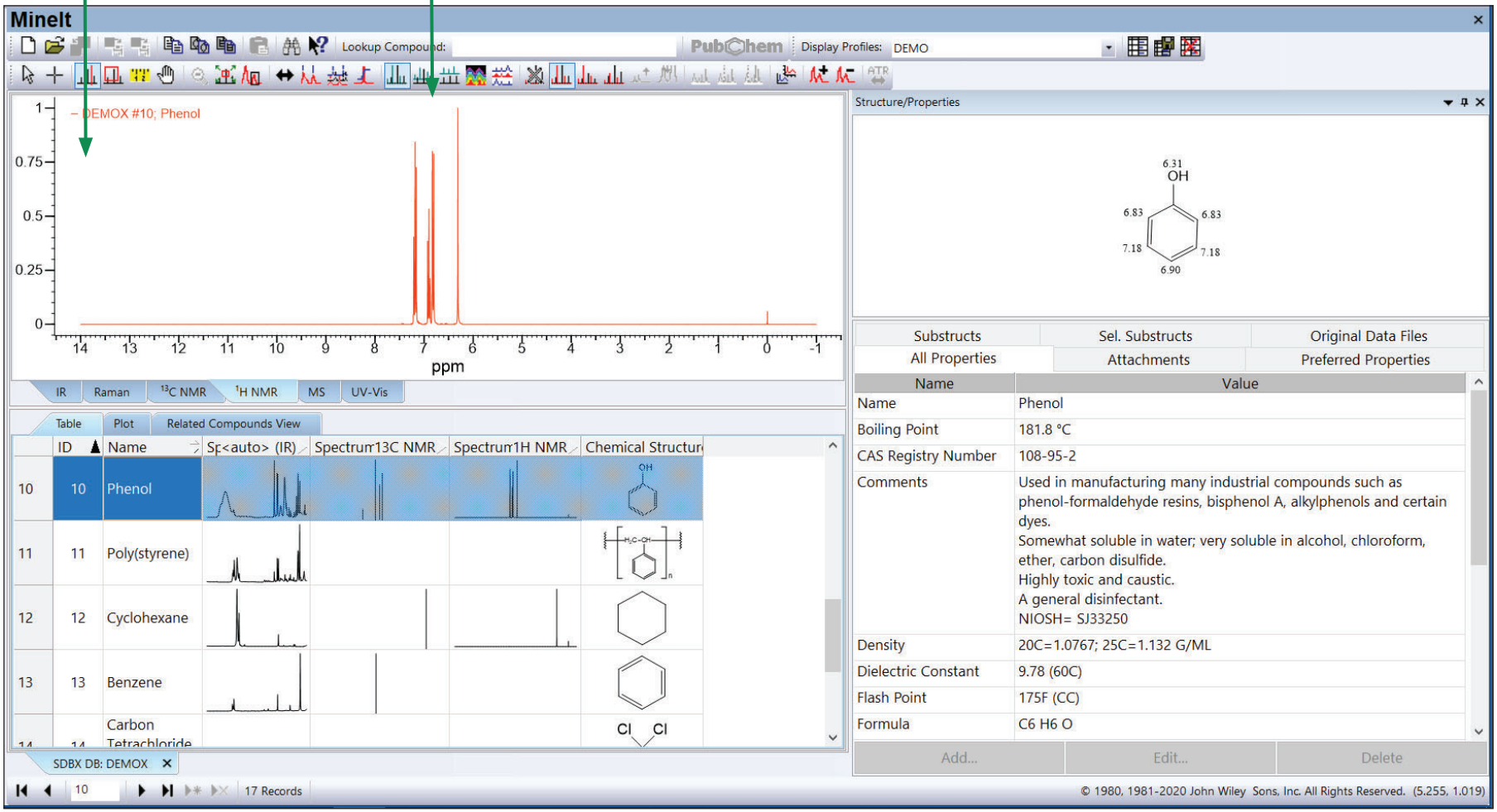
- IR, MS, NIR, NMR, Raman, UV-Vis
- Chromatograms
- Structures

Powerful Software + Quality Data. Results You Can Rely On.

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, improve workflow, and increase your ability to reach conclusions from your data.

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

Move seamlessly between tasks: search, process, manage data, draw structures, and more!



By combining tools and data into one system, you have greater ability to extract knowledge from your data!

What's Included?

Below is a bird's eye view of the tools and applications included.

Data Toolbox

ID Expert™	One-click spectral identification tool
SearchIt™	Advanced database searching
MineIt™	Spectral database building and data mining
QC Expert™	QC spectrum comparison
AssignIt™ NMR	Add assignments to databases

Spectral Analysis Toolbox

AnalyzeIt™	IR, Raman, IR Polymer functional group analysis
PredictIt™ NMR	NMR chemical shift prediction

Spectral Processing Toolbox

ProcessIt™	Spectrum processing for IR, MS, NMR, Raman; hyphenated MS processing

Basics Toolbox

ChemWindow	2D structure drawing
ReportIt™	Publish professional reports, with structures, spectra, chromatograms, etc.
BrowseIt™	Web portal with links to KnowItAll training resources and product news

Add-On Libraries

KnowItAll Spectral Libraries	Subscribe to the world's largest collection of IR, MS, NMR, Raman, UV-Vis

Explore the KnowItAll Tools In-Depth

- Data Toolbox
- Spectral Analysis Toolbox
- Spectral Processing Toolbox
- Basics Toolbox

KnowItAll ID Expert™

Spectral Identification for Basic Searches

When it comes to identifying unknown spectra, it's difficult to figure out where to begin. Wiley's KnowItAll ID Expert offers both novices and experts the perfect place to start. It provides fast, reliable answers to scientists identifying unknown spectra by matching against reference spectra.

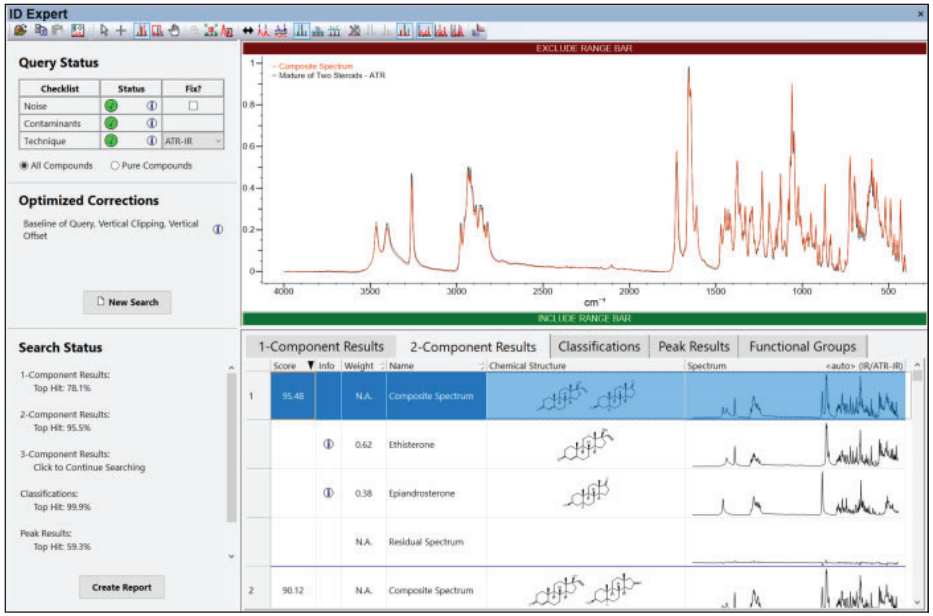
The spectral intelligence built into KnowItAll ID Expert when combined with Wiley's high-quality KnowItAll Spectral Libraries*—the world's largest collection—makes this a quick first pass tool.

How Does It Work?

- The user simply opens an unknown spectrum and KnowItAll ID Expert automatically performs a series of basic analyses—single and multi-component search, peak search, functional group (if IR/Raman)—and summarizes the results to give a complete overview of possibilities.
- If there are problems with the unknown spectrum or the reference spectra, ID Expert has the spectral intelligence to identify and fix some of these issues.
- Once the user has identified the unknown spectrum, a PDF report can be generated with a single click.

Includes Patented Optimized Corrections Technology to ensure best search results possible. Also includes quick classification for IR spectra of designer drugs using Wiley's new IR Designer Drug Models.

**KnowItAll Spectral Libraries require a subscription*



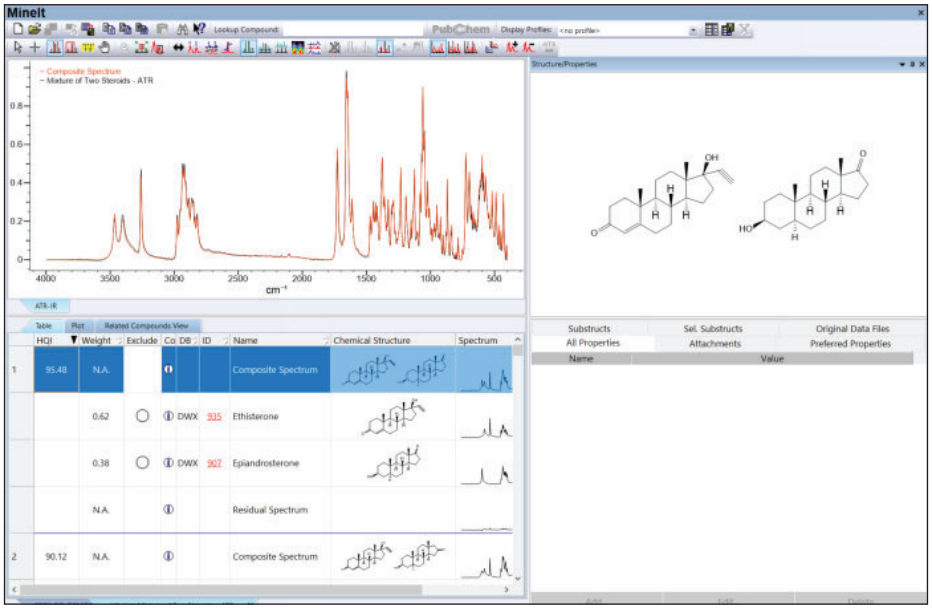
SearchIt™

For Advanced Spectral Database Searching

Wiley offers the most powerful tools to search spectral data, built using the same technologies Wiley uses to analyze its vast datasets. With fast search speeds, powerful algorithms, and patented technologies, Wiley is able to deliver results you can rely on.

Key Features

- Import sample spectrum and search against user-generated databases or KnowItAll spectral references libraries
- Searches are fully customizable and driven by powerful algorithms
- Optimized for speed and performance
- Search by name, structure, substructure, properties, spectra (full spectrum or selected range), and peak—in any combination
- Include or exclude regions from your search
- Perform mixture analysis for multiple components
- Include or exclude known components in mixtures to narrow results
- Manually select peaks or use automated peak picking capability
- Algorithms include Euclidean Distance, First and Second Derivative Euclidean Distance, Correlation, and Baseline Correction; For MS: Dot Product (Cosine), Wiley Dot Product (Cosine), Composite P1 and P3
- Perform simultaneous multi-technique search with spectra from various techniques to orthogonally validate for more confident analyses
- Includes patented Optimized Corrections technology to ensure best search results
- Includes MS Adaptive Search (patent pending) and Reverse Search
- Easily compare spectra using various views: overlay, offset, stack, butterfly, subtraction, etc.
- Supports multiple instrument types and vendor formats (see full list at www.knowitall.com/formats)



Powerful Spectral Analysis Tools that Set KnowItAll Apart

Wiley is committed to taking spectral analysis to the next level! We are continually adding spectrally intelligent tools to our portfolio that accelerate analysis. Here's a closer look at some of the unique and powerful solutions in **KnowItAll's SearchIt** that make Wiley a leader in spectral informatics!

Mixture Analysis: This industry leading capability for IR and Raman, is now available for MS! One of the most powerful features is KnowItAll's ability to analyze mixtures. When searching an unknown against a reference database, you can choose to search for multiple components. 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 (difference between the query and the composite spectrum). Composite spectra are then ranked by how closely they resemble the query spectrum.

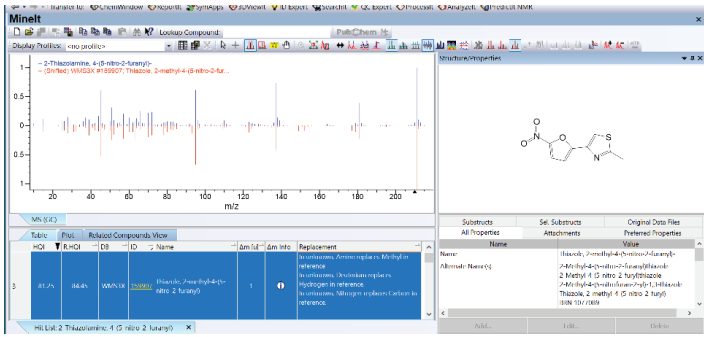
Patented Optimized Corrections Technology: Searching is not always a straight-forward process. What if there are problems with your query spectrum, library reference spectra, or both? If there is, you may never find the right match—even if it is in the library. Wiley offers a unique patented solution to solve this complex problem and lead you to the best results.

Wiley's Optimized Corrections is a spectrally intelligent solution built into KnowItAll's ID Expert and SearchIt applications. It performs a computationally complex set of corrections on all query and reference spectra in a search to find the optimal match between the query and each reference spectrum. Multiple corrections are applied automatically to compensate for differences between spectra caused by the variability of different instruments and accessories as well as other factors, including human error. Corrections include: baseline correction, clipping, horizontal shift, vertical shift, intensity distortion, and ATR correction.

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

NEW! Patent-Pending Adaptive Search for MS: When matching an unknown mass spectrum against a reference, this technology finds spectral matches that are similar to the unknown but have additional or missing selective fragment(s). It then suggests what might be causing the differences, where possible. This feature provides tremendous insight into structural possibilities to explore when there is no exact match. Ultimately, this may lead to more intelligent and confident identification and confirmation.

NEW! Reverse Search Feature: This search finds matches for peaks in the reference spectrum and ignores peaks which are only in the unknown spectrum.



MineIt™

Spectral Database Building and Management

Chemists and spectroscopists produce valuable data every day within their organizations. Because Wiley Science Solution's primary business is spectral databases, KnowItAll is built through years of experience in doing just that—building databases.

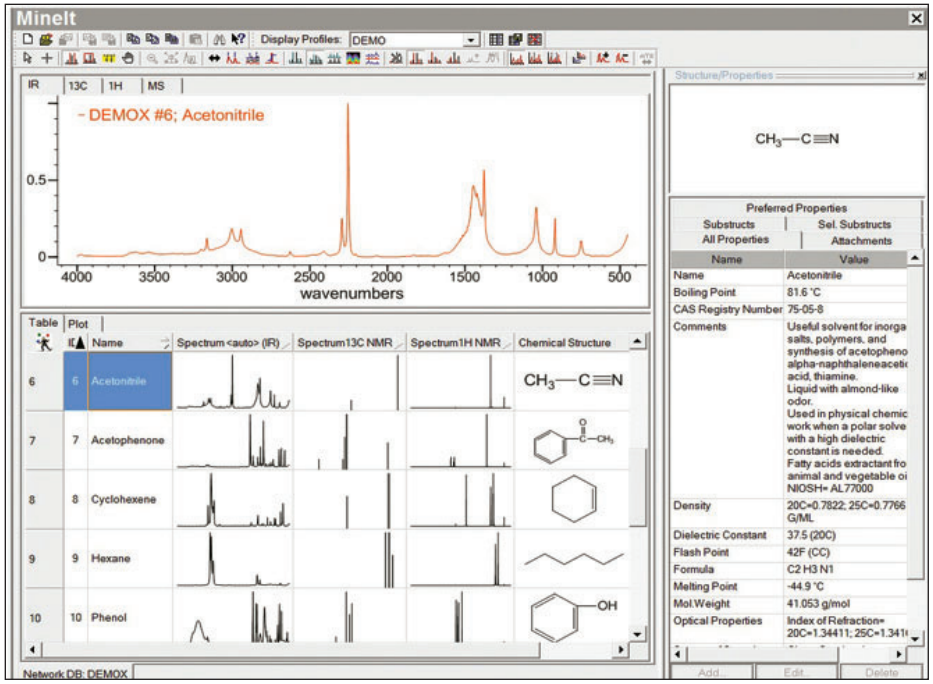
Build Single or Multi-Technique Databases from Various Vendors

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

Key Features

Build Databases with Spectral & Chromatographic Data

- Build databases with one or more analytical techniques
- Build databases with multiple spectral scans in the same record
- Import analytical data even if laboratory has instruments from multiple vendors
- One-click import of common instrument file formats or *.csv format (spreadsheet)
- Enhance each record with peak information, structures, and properties, such as source of sample, boiling point, etc.
- Import multiple structure formats (with stereo-chemical 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
- Make database more powerful by attaching spreadsheets, MSDS, and other documents or adding hyperlinks to web pages
- Create cross-reference from record to data from another technique; i.e., an NMR spectrum can be linked to an IR spectrum
- Property calculators for single or batch calculations for entire datasets - formula, molecular weight, C-13 NMR prediction, bad baseline indicator, baseline analysis: area difference, SPLASH ID, various masses (average, exact, nominal)
- MS tools to calculate elemental composition and isotope distribution
- Quickly add properties and structures from PubChem to your database



- Categorization of chemical structures of controlled substances according to Drug Enforcement Agency regulations

Customize Databases

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

Extract the Most Information from Your Data

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

Multi-Technique Viewing & Mining

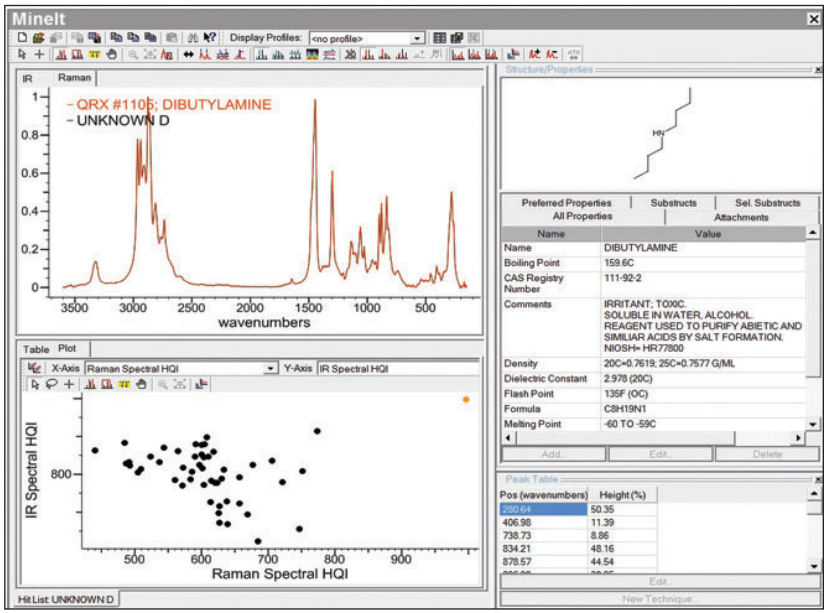
With MineIt, users can view reference databases, user-created databases, or search results. Access databases containing many types of data, such as spectra chromatograms, structures, physical properties, and more. Since analytical databases can contain one or more techniques in the same record, this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

Advanced Datamining Capabilities

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

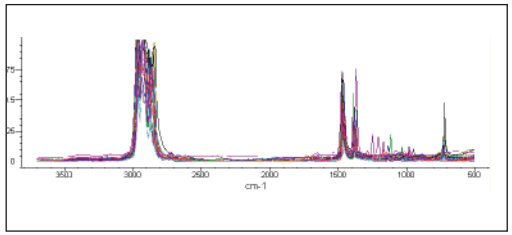
Patented Overlap Density Heatmaps Technology

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



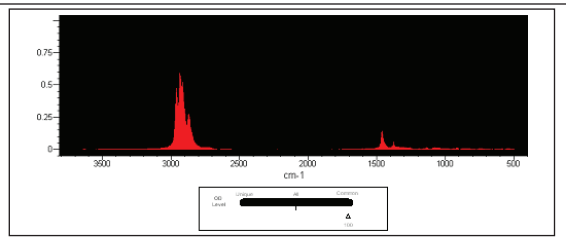
For example: This plotting feature is useful in the analysis of spectral searches for samples run in multiple techniques by plotting the quality of database search results (Hit Quality Indicies - HQIs) against each other (e.g., IR HQI versus Raman HQI).

Overlap Density Heatmaps: An Example



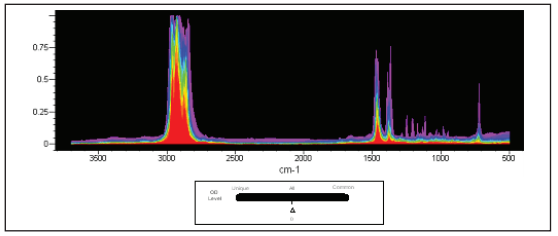
Traditional Stacked Display

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



OD Heatmap
OD Level = 100

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



OD Heatmap
OD Level = 0

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

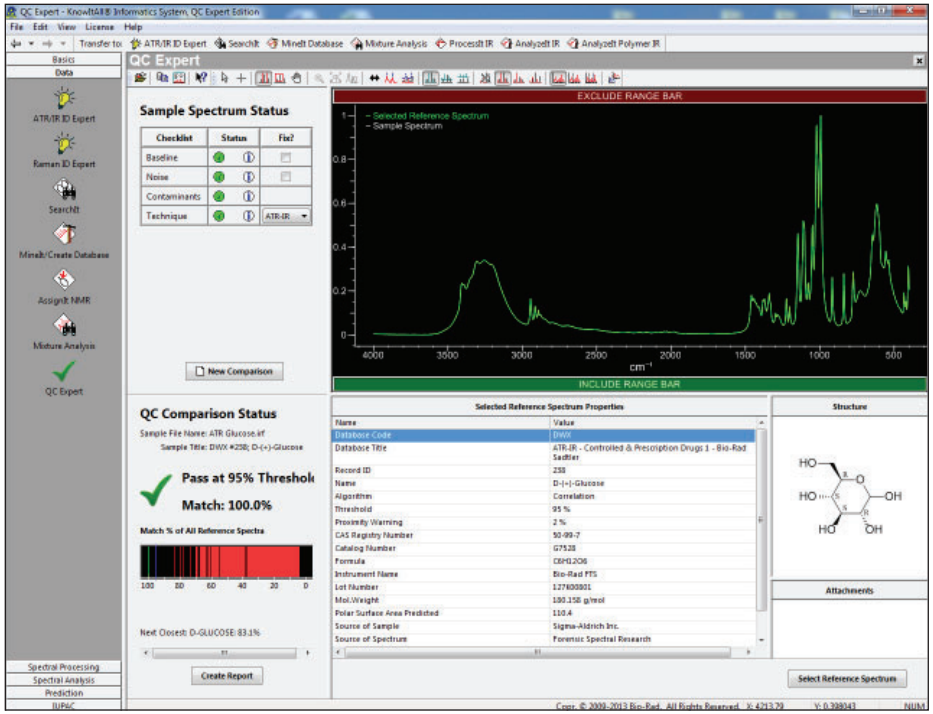
QC Expert™

IR & Raman Quality Control Comparison

Wiley'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



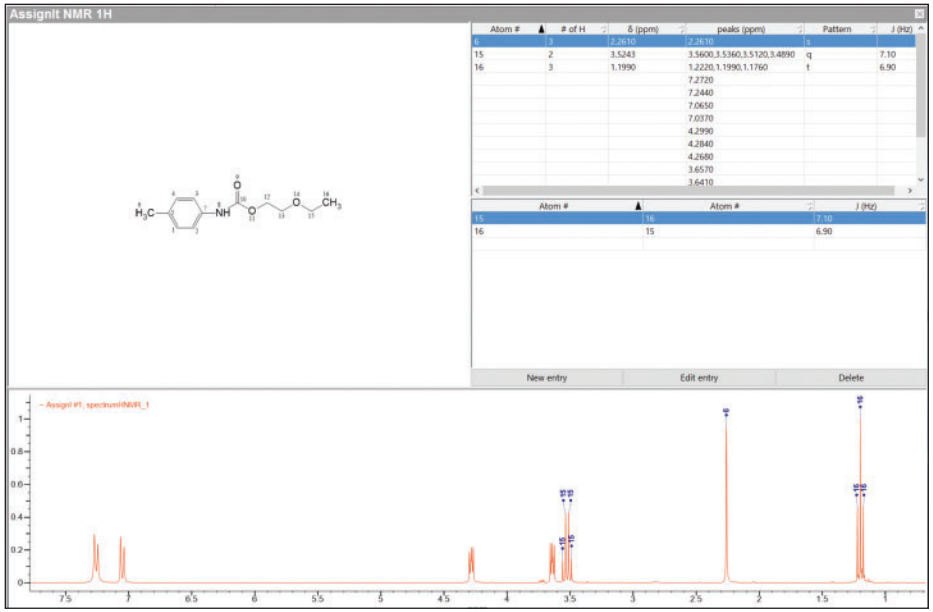
AssignIt™ NMR

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 ChemWindow (structure drawing) and MineIt™



Spectral Analysis Toolbox

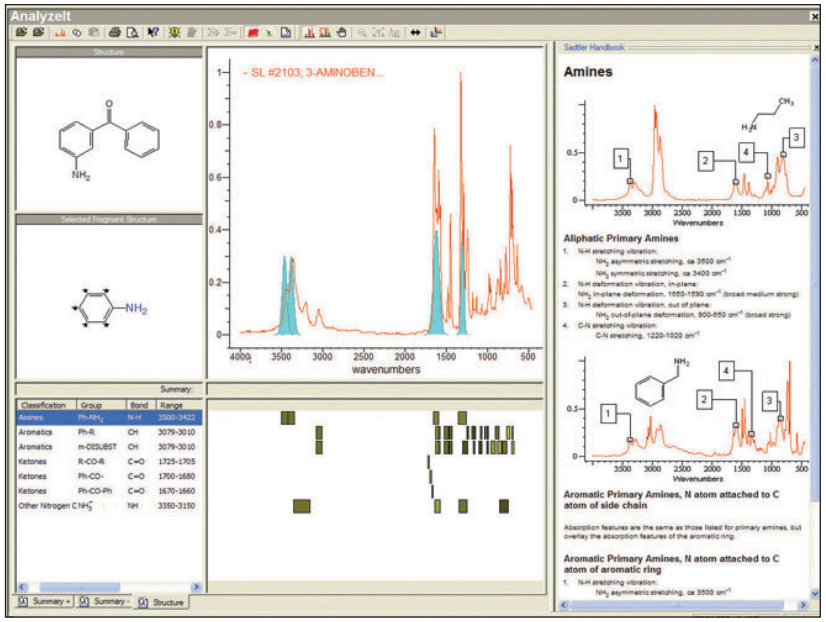
AnalyzeIt™

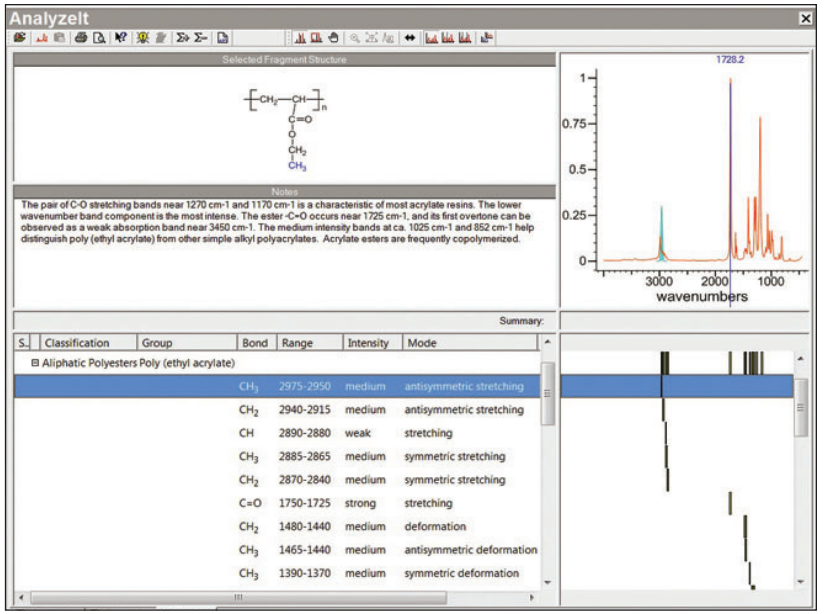
Advanced Functional Group Analysis for IR, IR Polymers, & Raman Spectra

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 proposed structure matches an observed spectrum. Just draw or import a structure to view its component functional groups. Then compare peak regions for each group by overlaying with the spectrum.

Build Your Own Knowledgebases: Improve interpretations by building knowledgebases of functional groups to use with AnalyzeIt's knowledgebase.





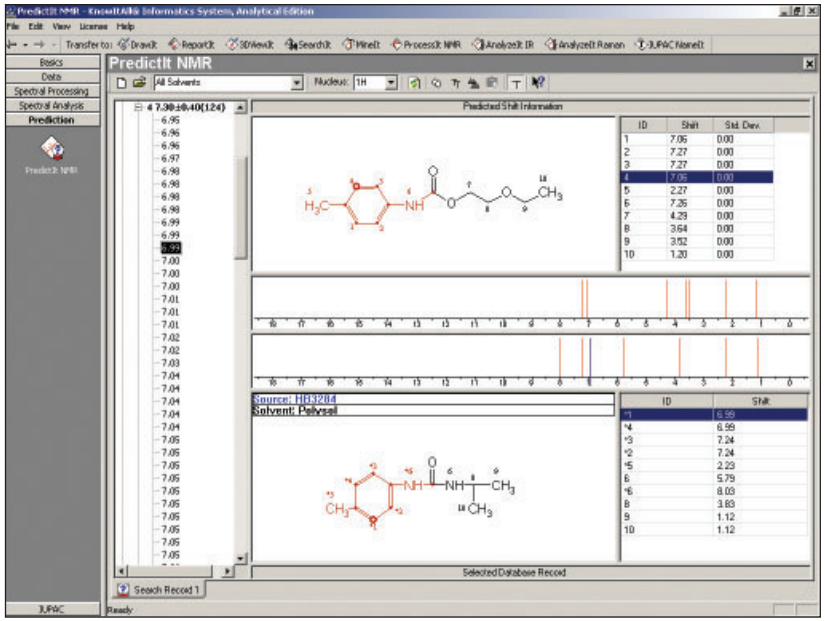
Benefits

- Useful in the identification of spectra of unknown compounds: IR, IR polymers, Raman
- Useful in classification/pattern characterization of chemicals
- Supplemental to other methods of spectral interpretation

Key Features

- IR/Raman knowledgebase of over 200 functional groups and hundreds of interpretation frequencies
- IR Polymer knowledgebase of over 100 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)
- View notes for functional groups when available

PredictIt™ NMR



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 users 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

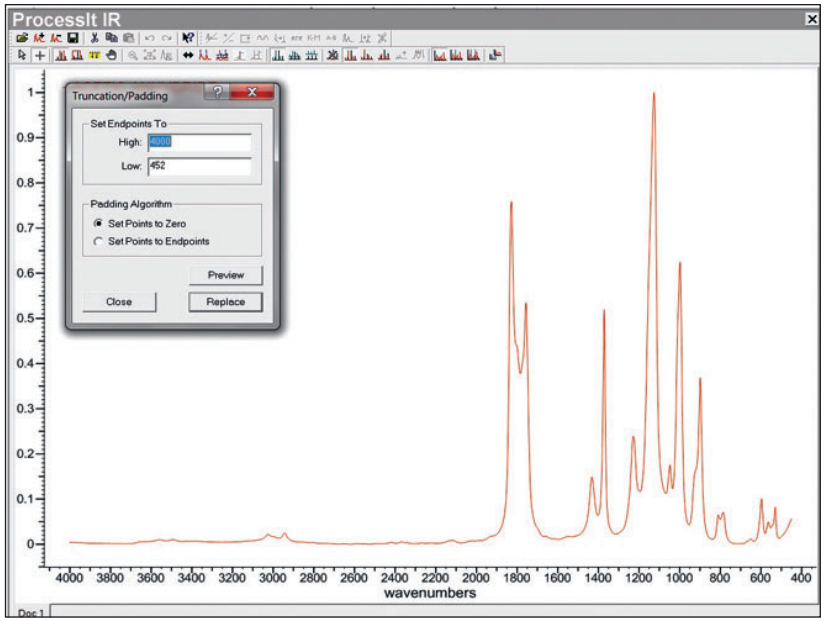
Predicted peak shifts are not the only piece of information that NMR spectroscopists need. PredictIt NMR not only allows easy retrieval of the real spectral data used to build the prediction, but also access to available information related to the reference spectrum, such as sample source, solvent, conditions of production, equipment, and properties for the molecule.

Spectral Processing Toolbox

ProcessIt™

IR Spectrum Processing

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



Processing Capabilities Include:

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

Analysis Capabilities Include:

- Area Under the Curve (AUC)

Raman Spectrum Processing

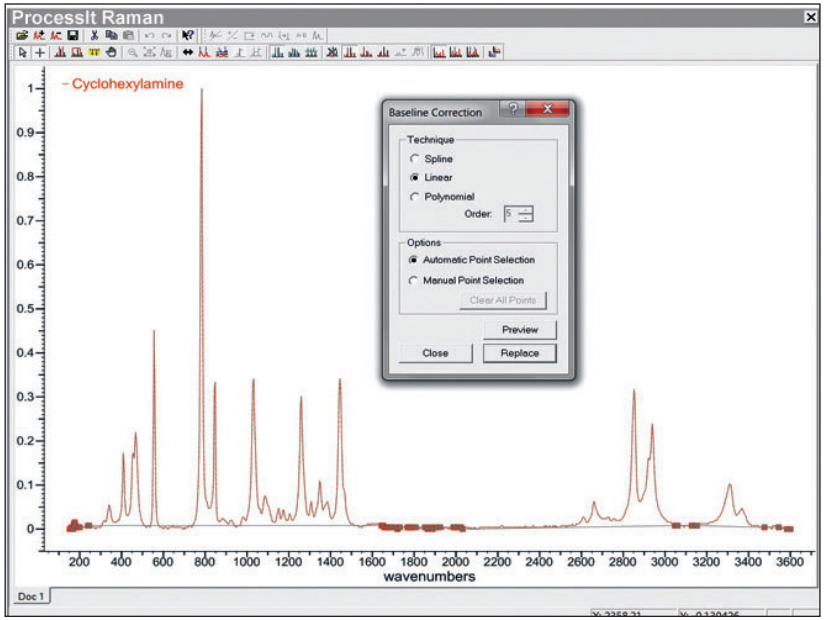
ProcessIt provides a number of tools to process Raman spectra and improve the quality of archived data and search results. It can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to ProcessIt to correct potential searching problems and transferred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

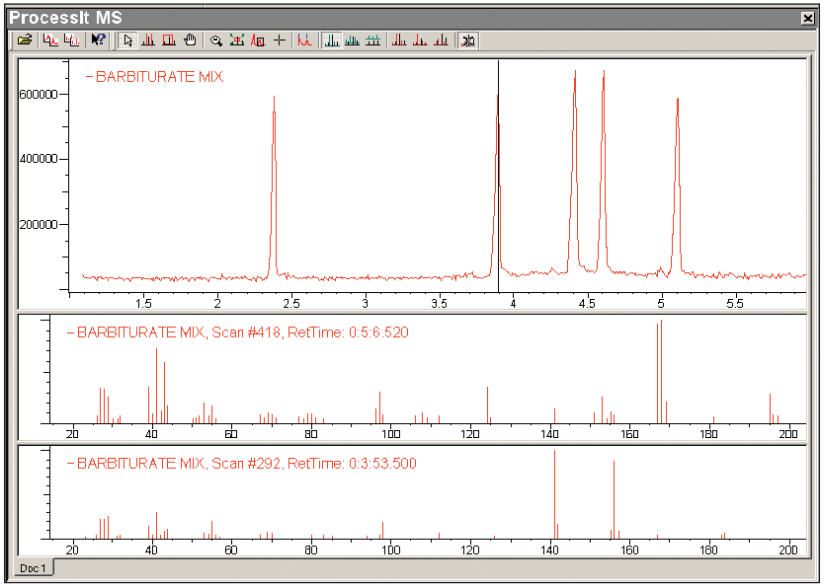
Processing Capabilities Include:

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

Analysis Capabilities Include:

- Area Under the Curve (AUC)





Mass Spectrum Processing

ProcessIt 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)

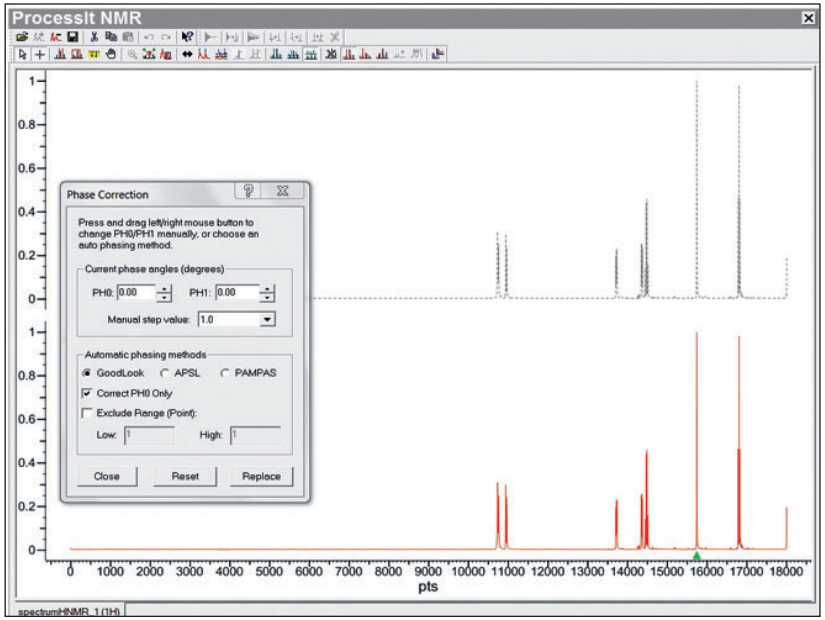
ProcessIt allows the display of a selected ion chromatogram in a different color. Multiple ion chromatograms can be displayed in the first pane. A selected ion chromatogram is very useful feature for verifying target molecules and determining whether the background profile is constant during the entire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

NMR Spectrum Processing

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



Key Features:

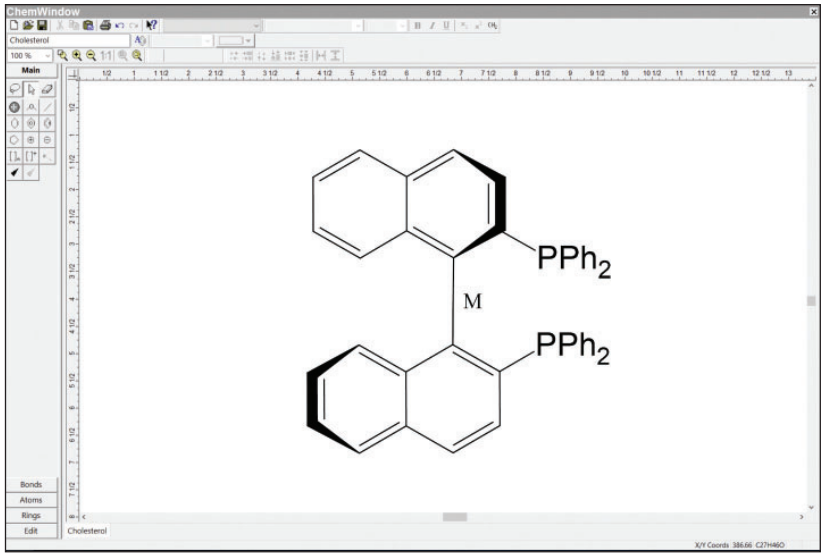
- Import 1D processed or FID spectra from multiple formats
- Processing features: zero filling, interactive window functions, and Fourier transform
- Automatic and manual phase correction
- Automatic and manual baseline correction, includes polynomial, spline and linear algorithms
- Automatic and manual 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

Basics Toolbox

ChemWindow®

A Full-Featured 2D Structure Drawing Program

ChemWindow is the software chemists worldwide choose for chemical structure drawing. It provides an advanced set of drawing tools that's easy to use— 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.



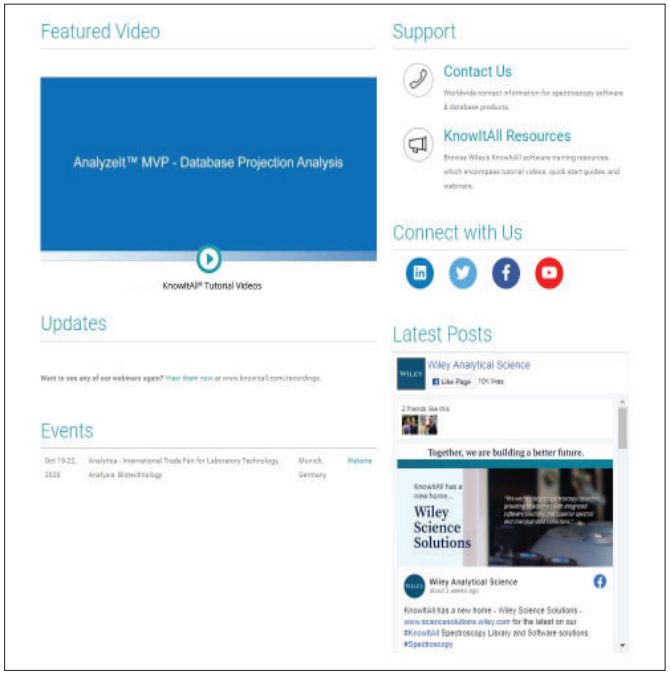
Key Features

- 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
- Advanced stereo-chemical recognition—using technology not available in other packages.
- OLE (Object Linking and Embedding) technology for in-place editing in word processing and presentation software
- Tools to calculate mass and formula, MS tools to calculate elemental composition and isotope distribution
- Predefined styles for captions and structures
- Links to OPSIN Name2Structure to convert a name to a structure
- Easily import existing structures from multiple file formats (ChemDraw - *.cdx, CML - *.xml, Hampden - *.hsf, InChI - *.txt, JCAMP - *.dx, *.jdx, BIOVIA/MDL - *.mol, *.rxn, Smiles - *.smi, XYX - *.xyz, etc.)
- Supports reaction files including RInChI, as well as CDX and CDXM files

BrowseIt™

Web Training Resources

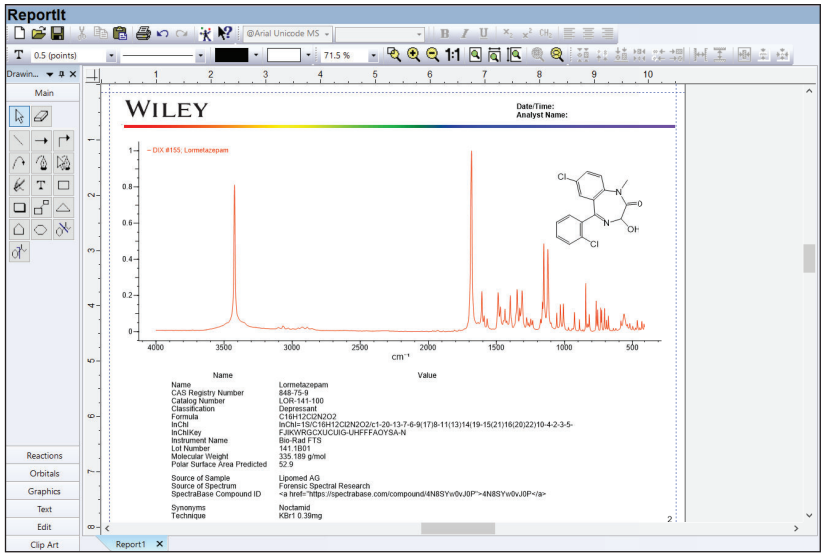
BrowseIt is a web browser built into the KnowItAll software with links to KnowItAll tutorial videos and other resources for KnowItAll users.



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 your data
- Spectrum / chromatogram import in common native file formats
- Multi-spectrum display in three display modes: overlay, stack, and offset
- Advanced spectrum display editing features to customize the appearance of spectra and chromatograms, including axes, colors, labels, etc.
- Custom annotation tool to link objects like spectral peaks to text graphics or chemical structure captions

KnowItAll Spectral Libraries

KnowItAll Software + the World's Largest Database

Wiley is the leading producer and publisher of spectral databases, with a collection that contains over 2 million spectra (IR, MS, NMR, Raman, and UV-Vis) covering pure compounds and a broad range of commercial products.

The KnowItAll software when combined with Wiley's KnowItAll spectral library subscriptions offers users an unparalleled solution for spectral identification. With access to massive collections of high-quality reference spectra, the likelihood and speed of analysis increases. It's that simple.

Ask about our subscriptions and other data options. Our experts can help you to determine the best data mix for your lab:

- KnowItAll IR Spectral Library
- KnowItAll Mass Spectral Library
- KnowItAll NMR Spectral Library
- KnowItAll Raman Spectral Library
- KnowItAll UV-Vis Spectral Library

Save Time & Resources

With an annual subscription, researchers get access to comprehensive collections of spectra—plus any updates. And with this much data, your laboratory can ultimately analyze samples faster and save valuable research time.

A Trusted Data Source for IR, MS, NMR, Raman, UV-Vis

Wiley is an authoritative source for spectral data. Their renowned Sadtler databases were processed according to rigorous protocols to ensure they are of the highest quality. These qualification procedures start at data acquisition and continue throughout the database development process. Any data acquired from trusted partners is thoroughly vetted before inclusion in our collections.

The KnowItAll collection is an essential tool for the identification, classification, and verification of unknown compounds in a wide range of applications such as polymer/materials, environmental, forensics/toxicology, pharmaceutical, biotech, automotive/aerospace, food/cosmetics, and many more.

Powerful Software + Quality Data. Results You Can Rely On.

sciencesolutions.wiley.com

REV20210817

WILEY