WILEY

KnowItAll Analytical Edition

Solutions to accelerate IR, MS, NMR, Raman, & UV-Vis analysis

POWERFUL SOFTWARE. QUALITY DATA.
RESULTS YOU CAN RELY ON.

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

Wiley's KnowItAll Analytical Edition offers solutions to **identify, analyze, and manage analytical data.**

Its vendor neutral environment **supports multiple instrument vendor file formats** and techniques to streamline your laboratory workflow and work the way you do.

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 **Wiley's comprehensive high-quality spectral reference databases***—including the renowned Sadtler libraries, Wiley Registry, Hummel, and spectra from trusted partners—KnowItAll gives chemists the most advanced technology available for fast, accurate analysis!

VPAT Compliant.
With accessibility features like keyboard access to menus, audio narration for icons, and tool tips.

Multi-language interface.
Software is currently available in English, Chinese, French, German, Japanese, and Korean.

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

KEY FEATURES

- Basic Spectrum Analysis
- Advanced Spectrum Search & Mixture Analysis
- Principal Component Analysis (PCA)
- Database Building / Management
- Structure Drawing & Reporting (ChemWindow)
- Spectrum Processing
- Comprehensive KnowItAll IR, MS, NMR, Raman, UV-Vis spectral library subscriptions available*

DATA TYPES

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

Tools for Technique-Specific Workflows- KnowItAll also incorporates custom tools for specific technique workflows such as IR/Raman functional group analysis, MS reverse & adaptive search (patented), automated MS deconvolution/analysis, NMR prediction & much more! Plus 12K bonus IR spectra.

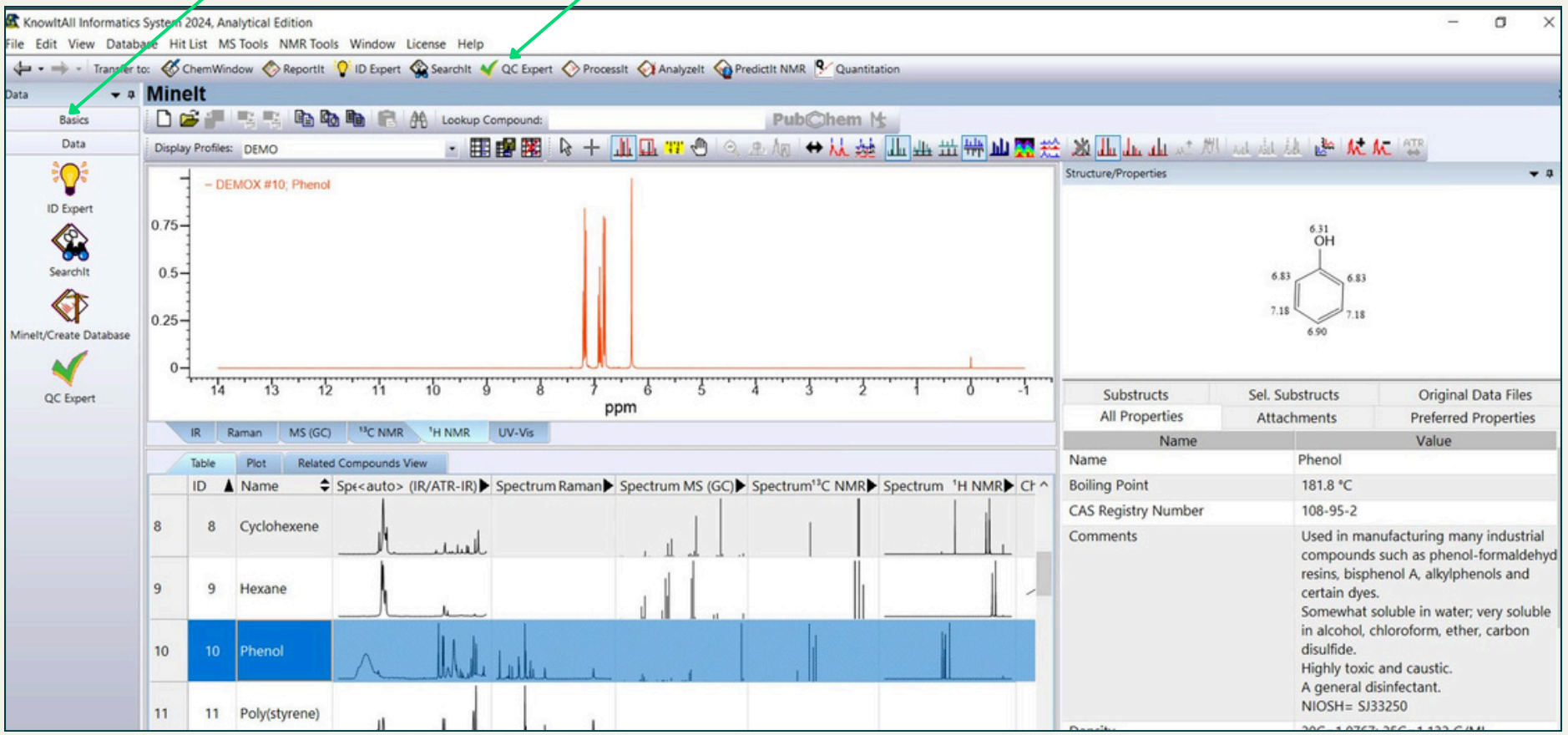
By combining all the tools and data you need into one system, you have greater ability to extract meaningful knowledge from your data.

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. Customizable toolboxes.

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



What's Included?

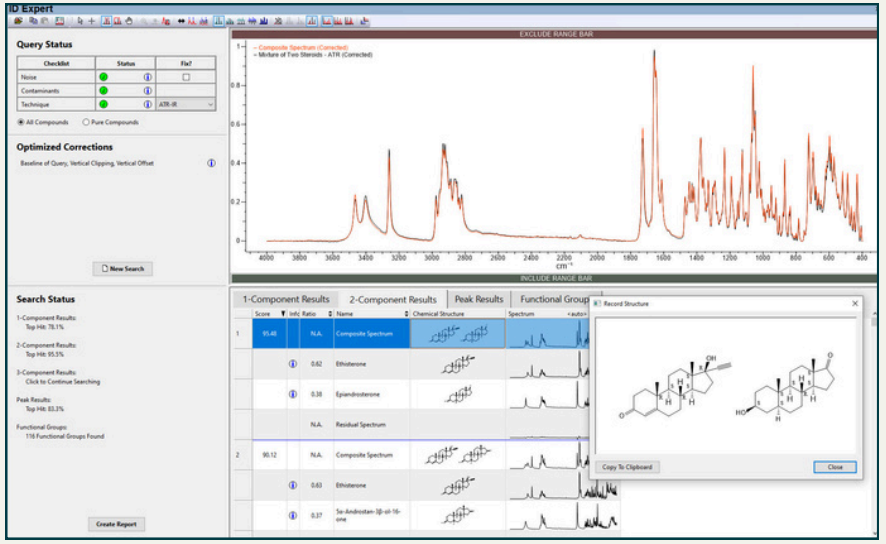
Snapshot of the tools and applications included.

DATA TOOLBOX	
ID Expert	One-click "first-pass" spectral identification tool
SearchIt	Advanced database searching
MineIt	Spectral database building and data mining
QC Expert	QC spectrum comparison
SPECTRAL ANALYSIS TOOLBOX	
Trendfinder	Discover hidden trends in data using principal component analysis (PCA) engine
AnalyzeIt	Functional group analysis - IR, Raman, IR Polymer, Vapor Phase IR Synthetic Cannabinoids
PredictIt NMR	NMR chemical shift prediction
SPECTRAL PROCESSING TOOLBOX	
ProcessIt	Spectrum processing for IR, NMR, Raman
GC Expert	Combines GC-MS deconvolution with automatic reference database search to analyze components
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
QUANTITATION TOOLBOX	
Quantitation	Support for internal and external standard workflows for GC-MS, IR, Raman, UV-Vis
OPTIONS	
LC Expert	Performs automatic non-targeted LC-MS/MS analysis and targeted accurate mass identifications
KnowItAll Libraries	Subscribe to comprehensive data collections of high-quality IR, MS, NMR, Raman, UV-Vis spectra

Explore the KnowItAll Tools In-Depth

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

KnowItAll ID Expert



First Pass Spectral Identification Tool

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 analysis 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.

If you have subscribed to Wiley's Drug Classification Models, you will be able to see the proposed classifications for your unknown spectrum here.

*Subscription required to KnowItAll Spectral Libraries.

SearchIt

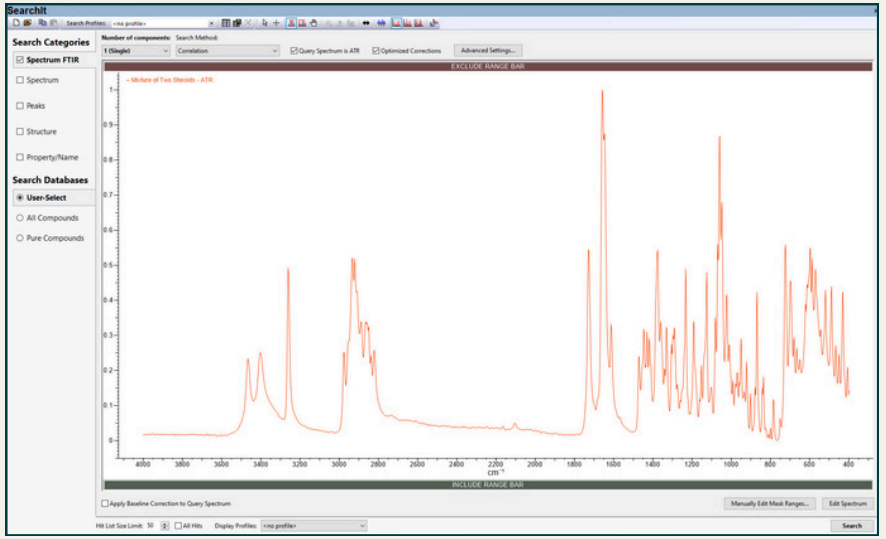
For Advanced Spectral Database Searching

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 comprehensive Wiley KnowItAll spectral references libraries for IR, MS, NMR, Raman, UV-Vis*
- 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 (patented), Reverse Search, and new Accurate Mass Search
- Easily compare spectra using various views: overlay, offset, stack, butterfly, subtraction, etc.
- Supports multiple instrument types and vendor formats (See supported formats: https://sciencesolutions.wiley.com/knowitall-supported-file-formats/)
- Ability to search Markush structures

*Subscription required to KnowItAll Spectral Libraries.



The Analytical Edition also includes these bonus databases:

- IR – Sadtler Polymers, Hummel – Wiley (1,907 spectra)
- IR – Sadtler Standards (Organic & Polymeric Compounds Subset) – Wiley (9,996 spectra)
- ATR-IR - Sadtler Solvents (629 spectra)
- **Microplastic Classifications Database** - This database is now included with the Analytical Edition as a fast and cost-effective way to classify microplastics of IR / ATR-IR spectra. For identification of microplastic samples, we recommend users subscribe to the comprehensive KnowItAll IR Spectral Library.

Powerful spectral search 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.

Patented 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.

MineIt™

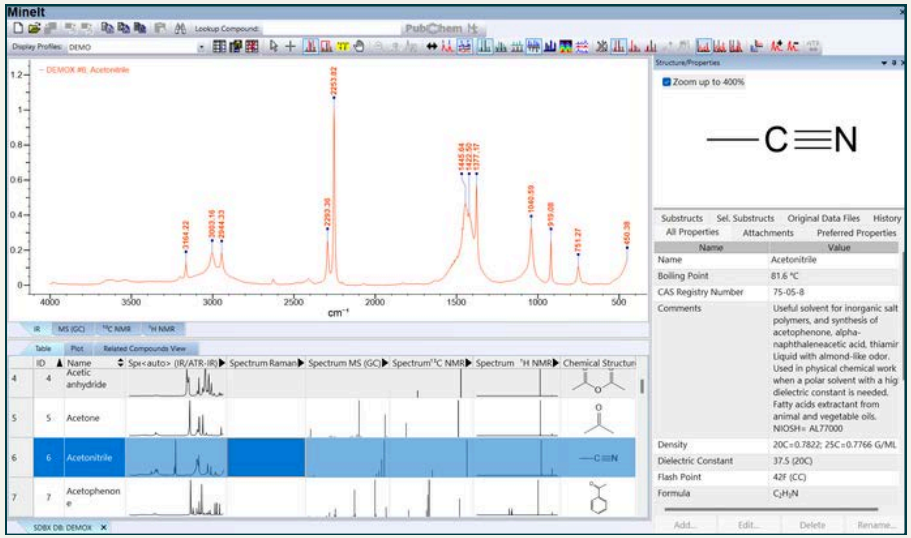
Spectral Database Building and Management

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 metadata. So even if a laboratory's instruments come from multiple manufacturers, KnowItAll can archive the data. (See supported formats: https://sciencesolutions.wiley.com/knowitall-supported-file-formats/)

Key Features
Build Databases with Spectral & Chromatographic Data

- Build databases with one or more analytical techniques
- Build databases with multiple spectra 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
- Categorize chemical structures of controlled substances according to *Drug Enforcement Agency* regulations (batch processing available)
- 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)
- Add peak labels to spectra
- Updated NMR tools for assigning multiplets to a structure and ability to automatically generate NMR reports for database records



- MS tools to calculate elemental composition and isotope distribution
- Quickly add properties and structures from PubChem to your database

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

Data Sharing

- Users can manage and share KnowItAll user databases created in their organization to extend the reach of these resources by using cloud storage services (e.g., AWS, Sharepoint, OneDrive, Google Drive, etc.).

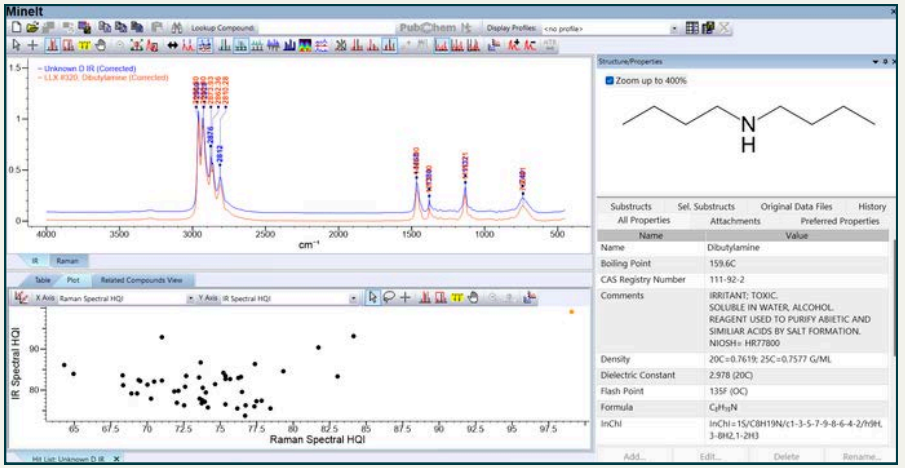
Data Control (Optional)

- Organizations can enhance the security and management of centralized, shared databases. Upon activation, organizations can connect to and utilize an Apache Subversion (SVN) repository to build shared KnowItAll databases, enabling robust version control and managed permissions.

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.

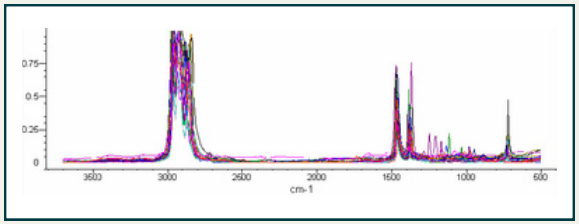
Advanced Datamining Capabilities
Compare any two variables from a database using a scatter plot diagram to separate data that follow a desired trend from that which does not. Select any point on the scatter plot to display the compounds associated with that record.

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.



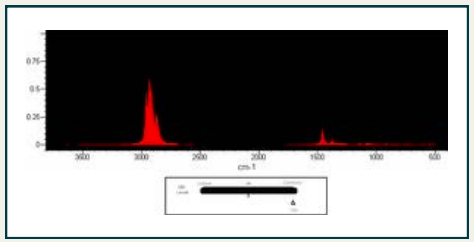
For example: This plotting feature is useful in the analysis of spectral searches for samples run in multiple techniques by plotting the quality of database search results (Hit Quality Indicies - HQIs) against each other (e.g., IR HQI versus Raman HQI).

OVERLAP DENSITY HEATMAPS: AN EXAMPLE



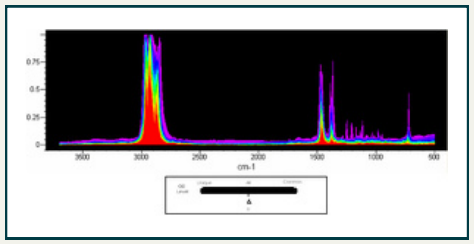
Traditional Stacked Display

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.

*Subscription required to KnowItAll Spectral Libraries.

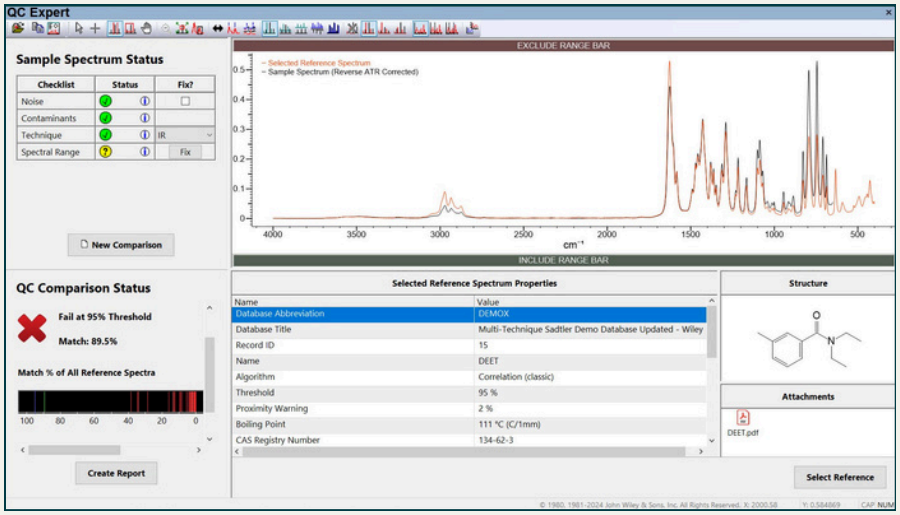
QC Expert™

IR, Raman, Chromatogram Quality Control Comparison

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

Key Features

- Perform QC comparison of a sample to a selected reference file
- Validate results by also comparing the sample to a reference database to ensure the sample not only matches the selected reference, but that it also does not match anything else in the reference databases*
- 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



*Subscription required to KnowItAll Spectral Libraries.

Spectral Analysis Toolbox

Trendfinder

Chemometric Data Analysis Simplified

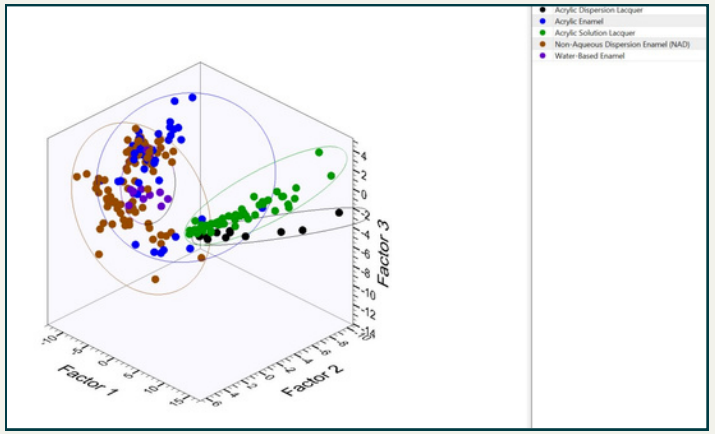
Discover hidden trends & patterns in large spectral or chromatographic datasets

New in KnowItAll 2026, Trendfinder applies Principal Component Analysis (PCA) to help you uncover meaningful patterns in complex datasets—whether you're working with spectra or chromatograms. It's designed to make trend detection and relationship mapping intuitive, even if you don't have a background in chemometrics. You can use your own data or tap into KnowItAll's vast spectral data collections* to explore correlations, outliers, and hidden structures that might otherwise go unnoticed.

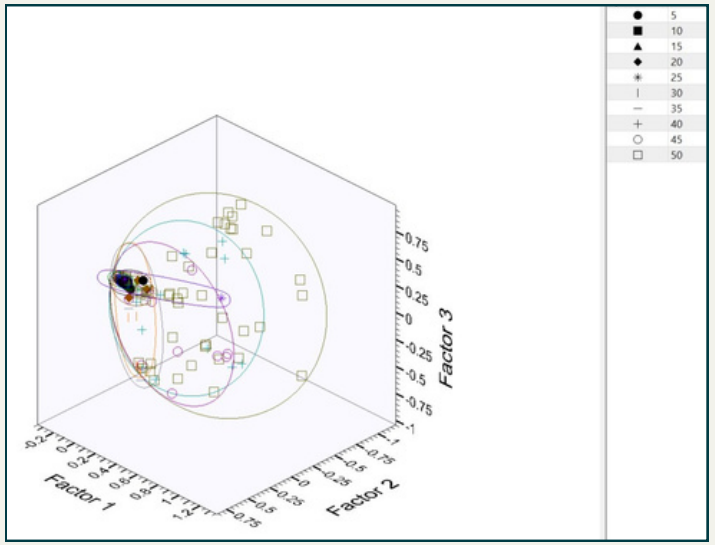
Key Features

- **Comprehensive dataset analysis:** Perform PCA on spectroscopic or chromatographic datasets
- **Expert-level analysis, user-friendly interface:** Advanced proprietary technology with intuitive visualization of relationships or trends
- **Unknown projection & discovery:** Classify unknown samples and identify markers
- **Comprehensive processing:** Complete suite of data preparation options without additional software (e.g., preprocessing, y-transforms, intelligent binning/bucketing, rotation)
- **Interactive Data Mining:** Various plots as integrated query devices for instant exploration
- **Multiple data sources:** Works with custom databases you build or bring into KnowItAll databases, or Wiley's vast datasets* (*Data subscription required)
- **Multi-technique capability:** Analyze data from various techniques - NMR, IR, Raman, MS, UV-Vis, chromatography
- **Seamlessly integrated:** Native integration within KnowItAll ecosystem eliminates data transfer issues

*Subscription required to KnowItAll Spectral Libraries.



This FTIR example shows PCA performed on a subset spectra from an automobile paint chips database. The legend on the right allows the user to select one or more properties by clicking on the appropriate row or rows in the legend.



This example shows a PCA analysis of tandem MS data. Higher collision energy spectra are spread out, and the lower collision energy spectra are clustered tight (black dots). This coincides with the fact that higher collision energies tend to break the molecules into smaller fragments, which makes the spectra differ more significantly from each other.

AnalyzeIt™

Advanced Functional Group Analysis

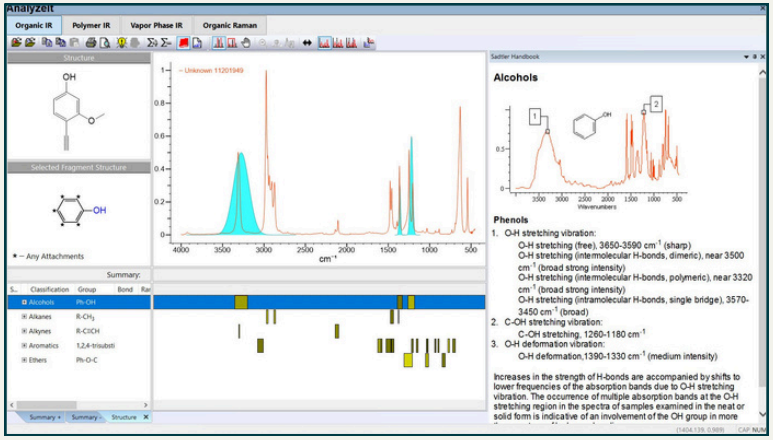
for IR, Raman, IR (Polymers), & Vapor Phase IR (Synthetic Cannabinoids)

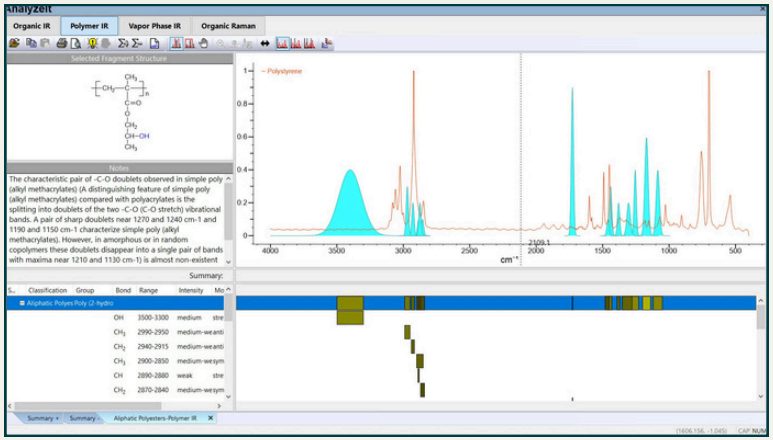
Interpret a Spectrum: Simply load a spectrum and click a peak of interest; AnalyzeIt then lists all functional groups possible at that peak position. Compare peak regions for each group by overlaying with the spectrum and narrow results by tagging the “most likely” candidates.

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.

CLASSIFICATION KNOWLEDGEBASES	
IR & Raman	Over 200 functional groups and hundreds of interpretation frequencies
IR Polymer	Over 100 functional groups and hundreds of interpretation frequencies
Vapor Phase IR - Synthetic Cannabinoids (Patented)	Over 60 bridge carbonyl groups

Or build your own knowledgebases to improve interpretations





Benefits

- Useful in the classification of spectra of unknown compounds
- Supplemental to other methods of spectral interpretation

Key Features

- 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
- Link to additional data in Sadtler Handbook (AnalyzeIt IR only)
- View notes for functional groups when available

PredictIt™ NMR

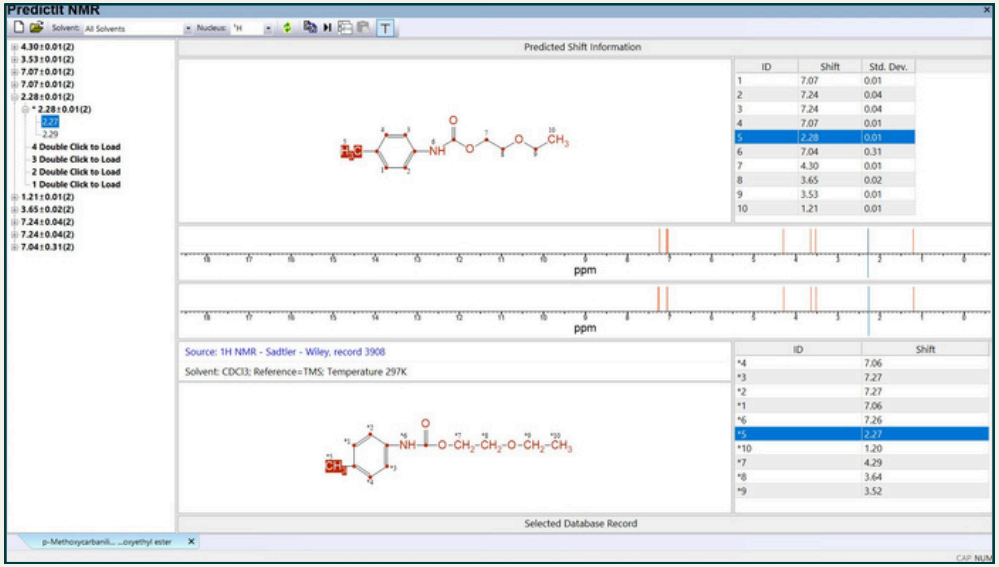
NMR Spectrum Prediction

With PredictIt NMR, perform database-based NMR spectrum predictions for ^{13}C, ^{1}H, and X-NMR 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 solvent-specific NMR chemical shift prediction. 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 and Raman Spectrum Processing

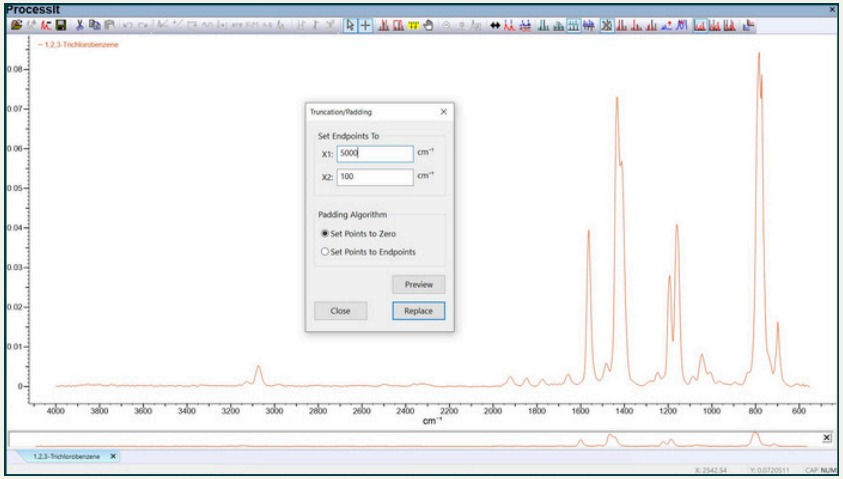
ProcessIt provides a variety of tools to process IR and Raman spectra and improve the quality of archived data and search results. It can also be used in conjunction with other KnowItAll tools. For example, a spectrum can be transferred from SearchIt to ProcessIt to correct potential searching problems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

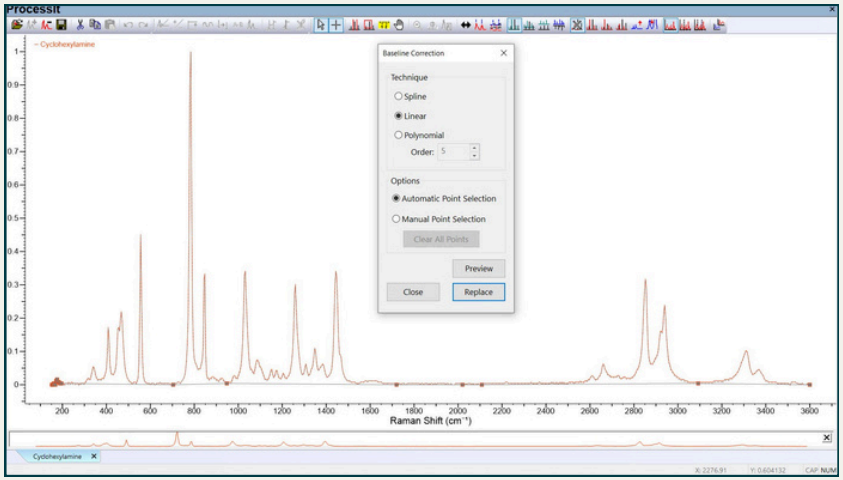
Processing Capabilities Include:

- 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
- Raman - Fluorescence correction
- Raman - Cosmic Ray removal
- Ability to add peak labels during processing that persist into your reports

Analysis Capabilities Include:

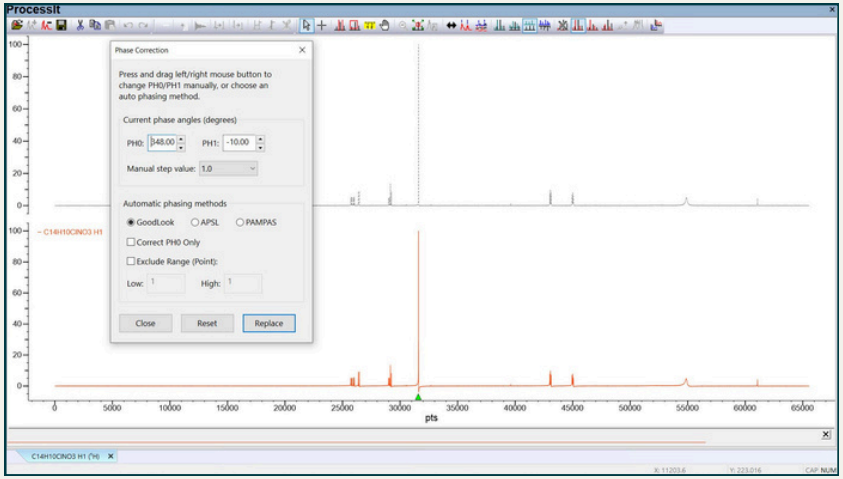
- Area Under the Curve (AUC)





NMR Spectrum Processing

ProcessIt is easy to use while offering a comprehensive set of processing features to correct experimental artifacts and improve the appearance of your spectra. Users have access to a full package of processing tools including pre-processing and post-transformation tools, as well as automatic and manual processing methods. KnowItAll's ProcessIt includes macro capability for repetitive workflows.



Key Features:

- Import 1D processed or FID spectra from multiple formats
- Processing features: zero filling, interactive window functions, and Fourier transform
- Phase corrections (automatic and manual)
- Baseline corrections (automatic and manual), includes polynomial, spline and linear algorithms
- Peak picking (automatic and manual)
- Integration (automatic and manual)
- Addition and subtraction of spectra
- Overlay multiple spectra for easy comparison
- Macro capability for quick and efficient processing
- Import and 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
- Ability to add peak labels during processing that persist into your reports

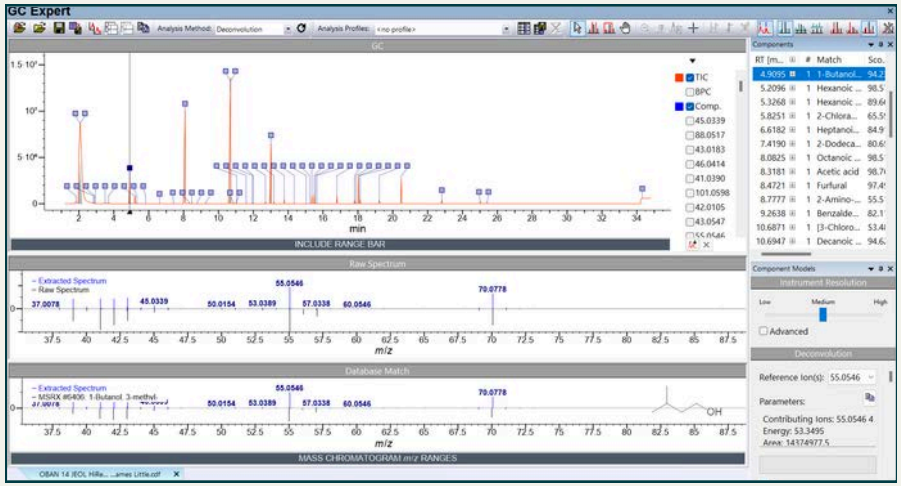
Multiplet analysis and structure assignment is available using MineIt's NMR tools.

GC Expert™

Non-Targeted GC-MS Analysis

GC-MS data analysis can be time consuming, especially when examining complex analytes. With GC Expert, automatically process, deconvolute, and analyze GC-MS data. Manual peak picking and analysis can also be performed. Combined with KnowItAll's fast database search, it suggests matches to known compounds and allows unknowns to be further examined.

When it is necessary to send coeluted components to the sophisticated mixture analysis application in KnowItAll, GC Expert facilitates this seamlessly. Novel compounds' structural characteristics can be further deduced by applying the patented MS Adaptive Search (in SearchIt) that uses fragmentation and structural information to propose probable structural details.



Key Features

- **Automatic processing:** Automatically process and deconvolute GC-MS data and search the extracted MS spectra to match against reference databases to identify components—all with a single click
- **Optimized for speed:** Fast, automatic database search built for speed
- **Comprehensive display:** Visualize TIC, component profile, extracted spectrum vs. raw spectrum, extracted spectrum vs. matched reference spectrum, and the matched reference component structure
- **Incorporate custom libraries:** Build in-house libraries using a proprietary database format that is optimized for spectral searches and retains raw data in its original format
- **Configure deconvolution and search settings:** Transition from automatic to manual deconvolution, with support for both unit and accurate mass datasets. Adjust analysis sensitivity parameters and configure the instrument resolution
- **Reuseable search profiles:** Create and reuse spectral search profiles that enable you to store preferred databases for a selected chromatogramic method
- **Seamless transfer to SearchIt for manual analysis:** Seamlessly transfer components which are not matched well to reference spectra to SearchIt for manual examinations using either Adaptive Search or mixture analysis. Adjustable match score calculations based on regular spectral search and reverse search HQI values
- **Broad compatibility:** Supports multiple instrument types and vendor formats (See supported formats: https://sciencesolutions.wiley.com/knowitall-supported-file-formats/)
- **Extensive database access:** Compatible with the comprehensive KnowItAll GC-MS spectral references libraries*
- **Integrated Reporting**: Send results direct to KnowItAll's integrated ReportIt tool to showcase your spectral identification results, complete with spectra, structures, annotations, data tables, and more

How Does It Work?

Simply import a GC-MS data file and the software automatically deconvolutes the TIC into components. All extracted component MS spectra are then automatically searched against reference libraries* to find matches. Results are shown as a hit list for each component.

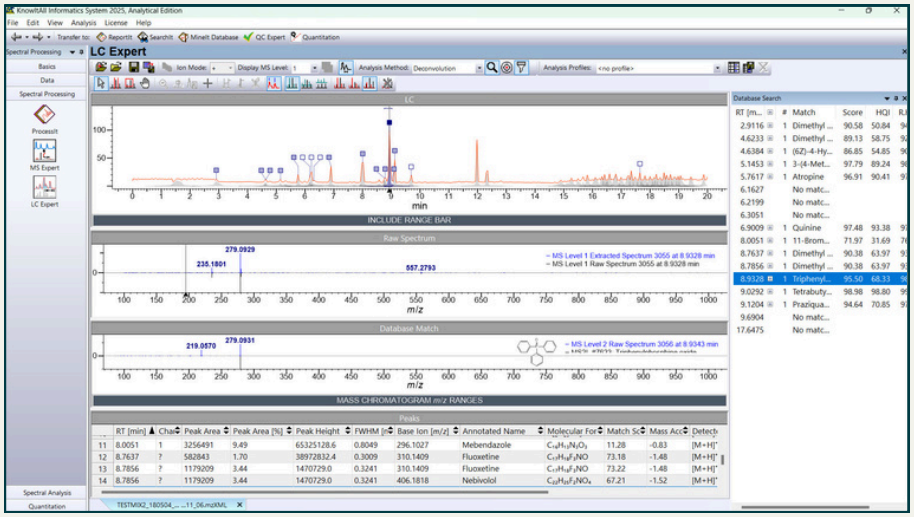
Unidentified components or components with low match scores can then be sent to KnowItAll's SearchIt tool for manual investigation. In SearchIt, one can use adaptive search to match similar components or use mixture analysis to separate coeluted components.

*Subscription required to KnowItAll Spectral Libraries.

LC Expert™ (Option)

Streamline component identification with the power of LC Expert's automated workflow

LC-MS data analysis can be time consuming and tedious. The new LC Expert rises to the challenge with an automatic workflow that processes, deconvolutes, and searches raw LC-MS chromatograms. LC Expert features both MS/MS and accurate mass search methods for the most complete analysis. Combined with the power of KnowItAll's comprehensive, high-quality database collections*, LC Expert takes non-targeted and targeted spectral analysis to the next level.



Key Features

- **Automatic processing:** Automatically process and deconvolute raw chromatograms and search against reference databases to identify compnents—all with a single click
- **Optimized for speed:** Fast, automatic database search built for speed
- Comprehensive display: Visualize TIC, component profile, extracted spectrum vs. raw spectrum, extracted spectrum vs. matched reference spectrum, and structure for the database match
- **Incorporate custom libraries:** Build in-house libraries using a proprietary database format that is optimized for spectral searches and retains raw data in its original format
- **Configure deconvolution and search settings:** Adjust analysis sensitivity parameters and configure to the instrument resolution. Support for both unit and accurate mass datasets
- **Reuseable search profiles:** Create and reuse spectral search profiles that enable you to store preferred databases for a selected chromatogramic method
- **Seamless transfer to SearchIt for manual analysis:** Seamlessly transfer components which are not matched well to reference spectra to SearchIt for manual examinations using either Adaptive Search or mixture analysis. Adjustable match score calculations based on regular spectral search and reverse search HQI values
- **Access to the renowned MSforID search algorithms:** Use this algorithm to leverage the power of databases containing multiple collision energy measurements per compound
- **Broad compatibility:** Supports multiple instrument types and vendor formats (See supported formats: https://sciencesolutions.wiley.com/knowitall-supported-file-formats/)
- **Extensive database access:** Compatible with the comprehensive KnowItAll LC-MS spectral database collection and many other popular MS/MS libraries also offered in KnowItAll format
- **Integrated Reporting:** Send results direct to KnowItAll's integrated ReportIt tool to showcase your spectral identification results, complete with spectra, structures, annotations, data tables, and more

How Does It Work?

Import an LC-MS chromatogram data file and the software automatically deconvolutes the TIC into peaks. All peaks are integrated and tabulated. If the dataset contains tandem MS data, the raw MS/MS spectra are automatically searched in the preselected LC-MS libraries*. Users are also able to perform accurate mass searches for lists of known target compounds.

*Subscription required to KnowItAll Spectral Libraries.

Basics Toolbox

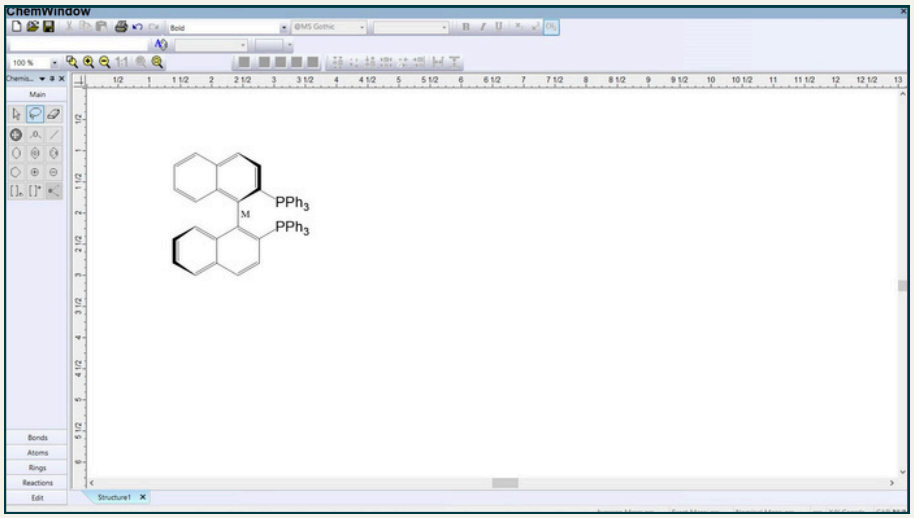
ChemWindow®

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

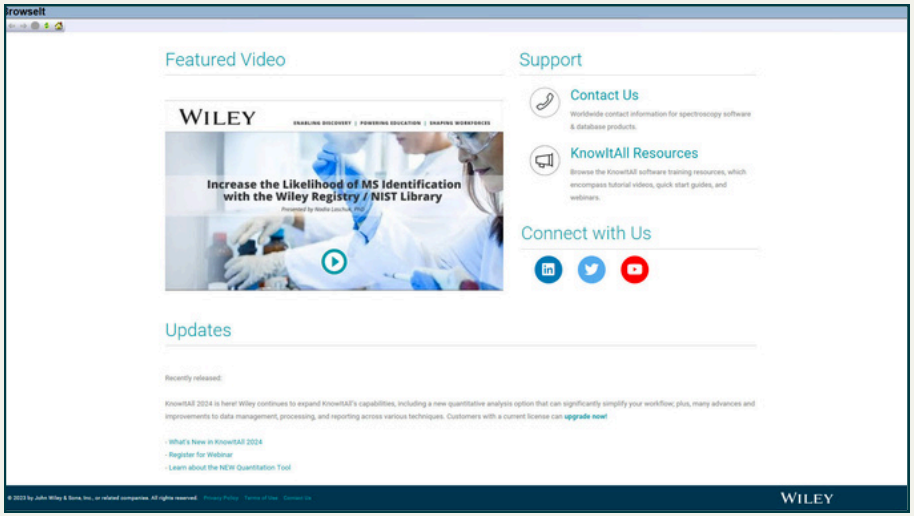
- Customizable toolbars with tools to draw chemical structures, including bonds, rings, atom labels, charges, etc.
- Chemical recognition features such as hot keys, chemical syntax checker
- Advanced stereo-chemical recognition—using technology not available in other packages.
- OLE (Object Linking and 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, CDXML - *.cdxml, 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 CDXML files
- Represent definitions of complex chemical classes using Markush type structures



BrowseIt™

Web Training Resources

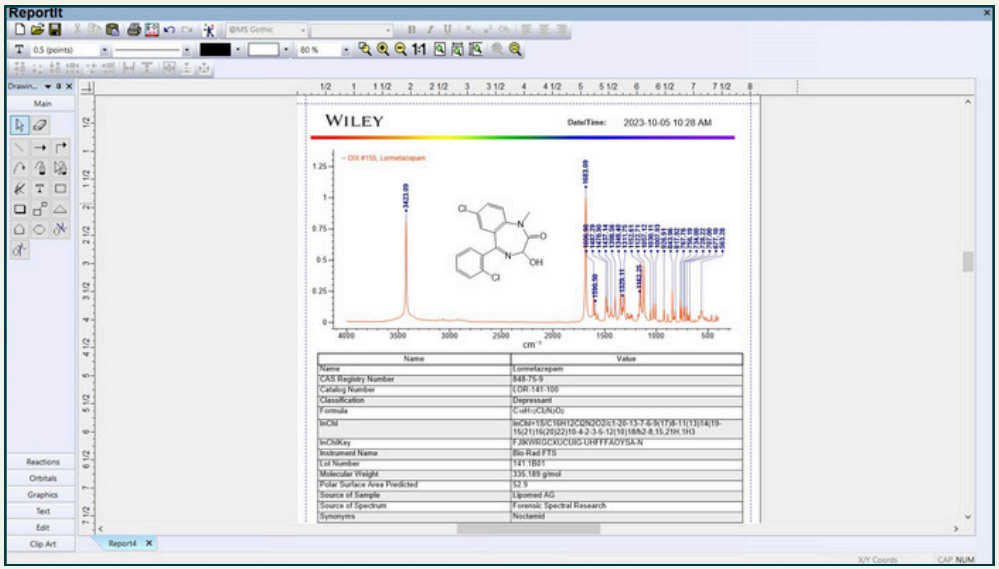
- BrowseIt is a web browser built into the KnowItAll software with links to KnowItAll tutorial videos and other resources for KnowItAll users



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

Quantitation Toolbox

Quantitation

Quantitation

Quantitation

A Quantitative Analysis Tool

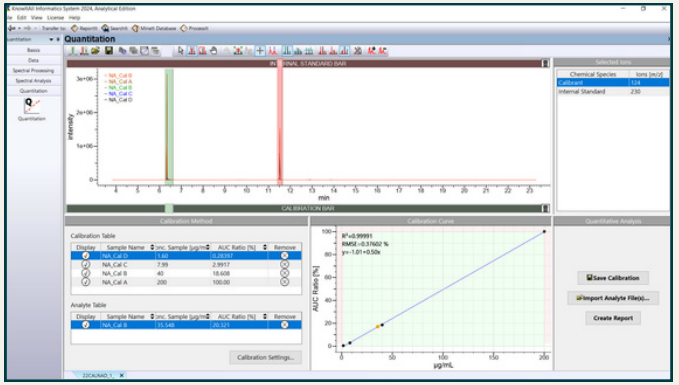
Wiley's KnowItAll has always helped us to answer "what" the identity of a substance is. Now you can answer "how much" substance there is with an integrated quantitation tool, **to complete and simplify your analytical workflow.**

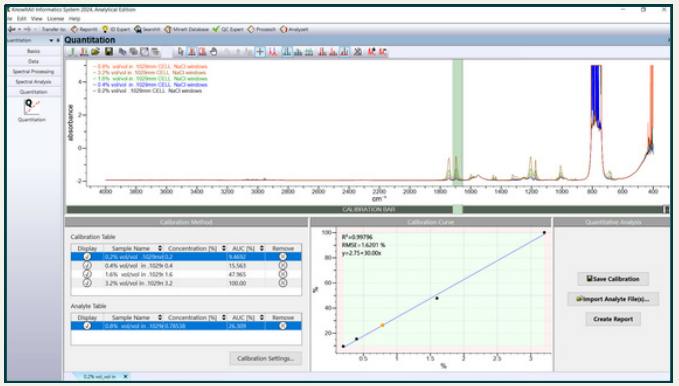
When it comes to chemical quantitative analysis, researchers often find themselves navigating multiple software packages. Mastering multiple software packages to achieve the same level of expertise, reproducibility, and interoperability is a major pain point and a training challenge. Further disruptions to analysis occur when lab personnel are forced to switch tools, or cut and paste between packages, depending on the type of analytical technique or data format.

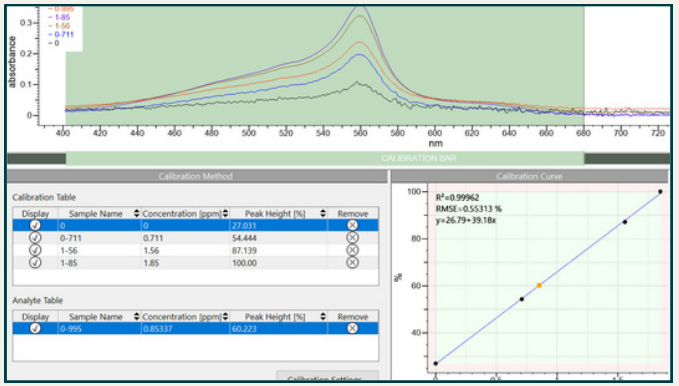
To overcome these challenges, Wiley's new KnowItAll Quantitation Tool provides a single, easy-to-use tool to perform these tasks consistently in a vendor-neutral environment that supports multiple techniques (GC-MS, IR, Raman, UV-Vis, GC) and instrument formats.

Key Features

- Unlike other packages, KnowItAll quantitation supports multiple techniques and vendor formats. Currently, suitable for **GC-MS, IR, Raman, UV-Vis, GC.**
- It is intuitively designed, providing a **simple step-by-step walkthrough** process in a single interface.
- Methods include: **external calibration, internal calibration,** and **standard addition analysis.**
- There is **no need to switch to tools outside your analytical workflow** like excel that require manual processes and are hence prone to error. It even allows for data input directly from tables from which the values are extracted.
- Moreover, because the tool is integrated with familiar KnowItAll interface, it **shortens the learning curve**.
- Access to essential mathematical operators for quantitation analysis **including linear and quadratic regression**, add **weighting to fit**, and **force line through origin.**

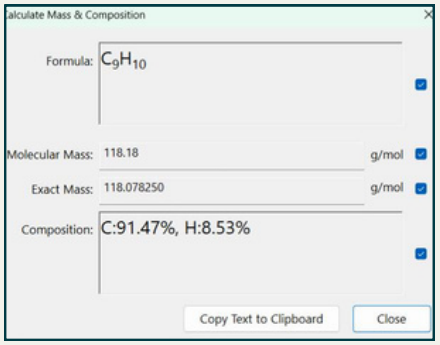




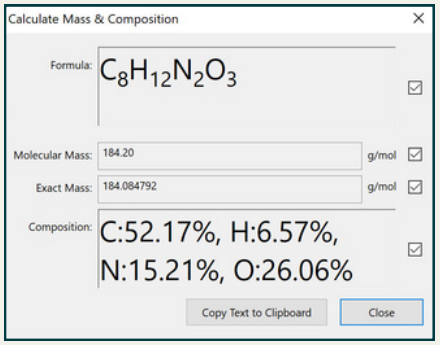


Additional Tools

Chemistry Tools

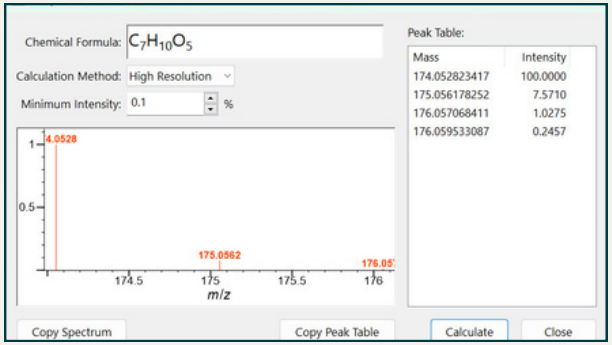


Calculate Mass & Composition. Automatic calculation of molecular mass, exact mass and composition from a chemical formula.

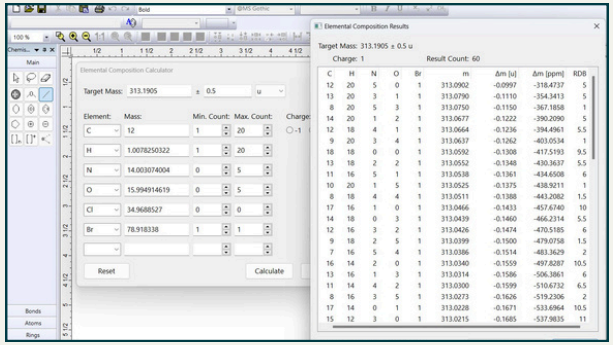


Formula Calculator. Automatic and tunable calculation of molecular weight, moles, and mass from chemical formula.

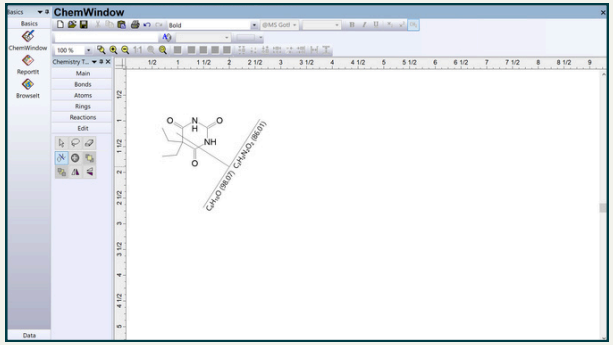
MS Tools



Isotopic Distribution Calculator. Calculate the isotopic distribution from a chemical formula using either low resolution or high resolution to a user defined threshold.



Elemental Composition Calculator. Calculate possible chemical formulas from target mass and sample elements.



Fragmentation Tool. Predict the m/z value for mass fragments in MS from a structure.

Accelerate Your Analyses with KnowItAll Spectral Libraries

From the Leader in Spectral Data

Spectral analysis software is not complete without a high-quality database of reference spectra. And with KnowItAll, Wiley offers the best of both!

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

Analyze Samples Faster
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. Your lab can ultimately analyze samples faster and save valuable research time.

Broad Compound Coverage
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.

Trusted Data from a Trusted Source
Wiley is an authoritative source for spectral data. Their renowned databases are 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.

OUR EXPERTS CAN HELP YOU DETERMINE THE BEST DATA MIX FOR YOUR LAB

- KnowItAll IR Spectral Libraries
- KnowItAll GC-MS Spectral Libraries
- KnowItAll LC-MS Spectral Libraries
- KnowItAll NMR Spectral Libraries
- KnowItAll Raman Spectral Libraries
- KnowItAll UV-Vis Spectral Libraries
- KnowItAll SmartSpectra Libraries

With KnowItAll annual subscriptions, researchers can get access to comprehensive collections of spectra—plus updates available.

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

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