WILEY

KnowItAll ChemWindow Edition

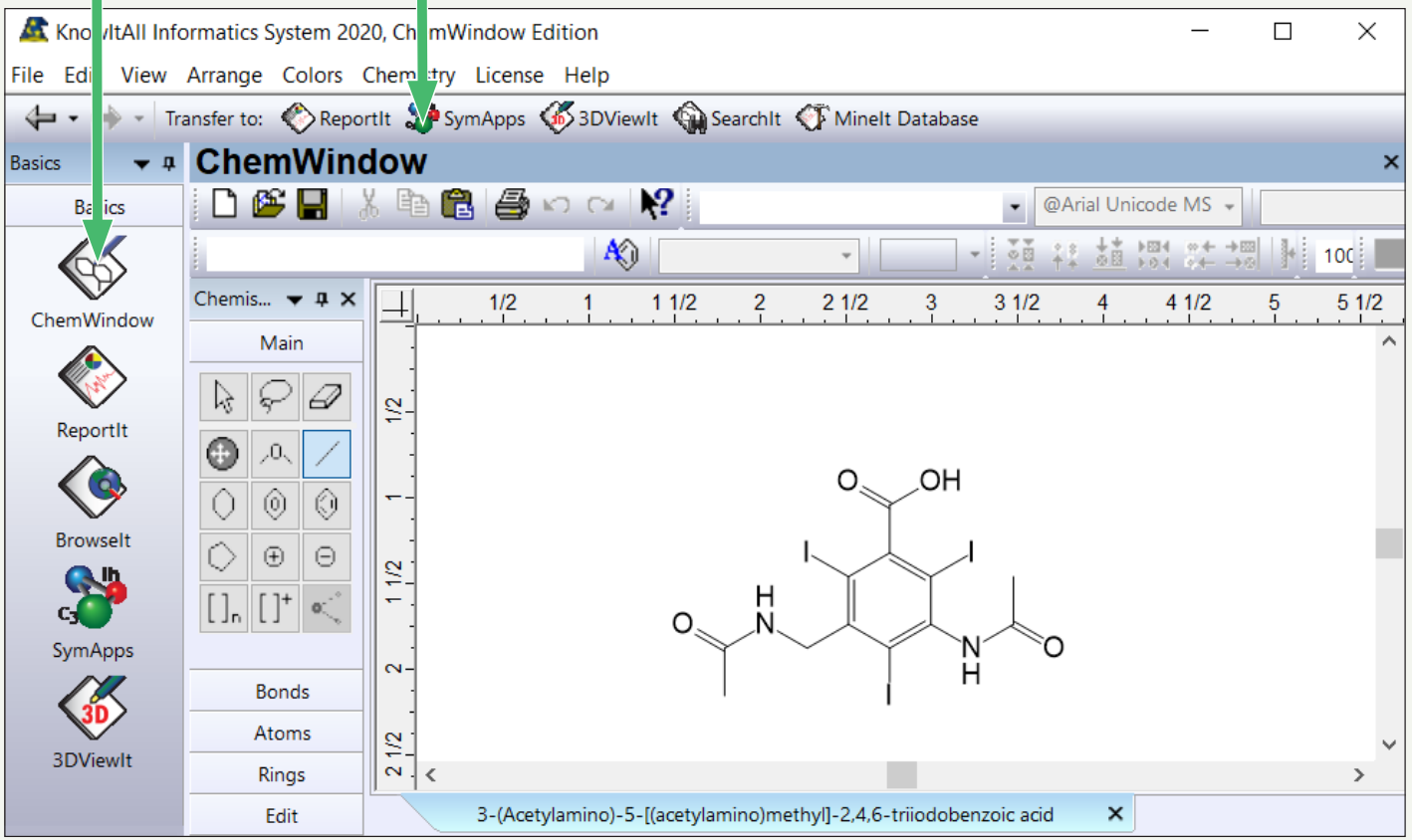
Software for Structure Drawing,
Data Management, & More

Draw Structures. Create Reports. Manage Data.

Wiley's KnowItAll, ChemWindow Edition is the software chemists choose for chemical structure drawing and publishing worldwide. Now with integrated solutions to modify, store, search, and retrieve chemical structures and properties, ChemWindow offers scientists even more solutions.

Versatile Toolboxes.
Draw structures, publish reports & more.

True Integration.
Instantly transfer data from one application to another.



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.

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What's Included?

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 **shorten the learning curve**.

BASICS TOOLBOX

ChemWindow®	2D structure drawing (includes advanced stereo-chemical recognition not available in other packages)
ReportIt™	Publish professional reports, with structures and more
SymApps™	3D presentations and 3D modeling, plus calculation of point groups, bond lengths, angles, etc.
3DViewIt™	Visualization of 3D structures
BrowseIt™	Web portal with links to training resources and product news

DATA TOOLBOX

SearchIt™	Database searching (search structures, properties)
MineIt™ / Database Building	Database display and mining; build databases with structures and properties

ADDITIONAL FEATURES

Clip Art Libraries	Laboratory Glassware and Chemical Engineering collections
Calculation Tools	Calculators for easy mole-to-mass conversion and calculation of mass from structure
MS Fragmentation Tool	Determine whether your proposed structure matches your mass spectral data

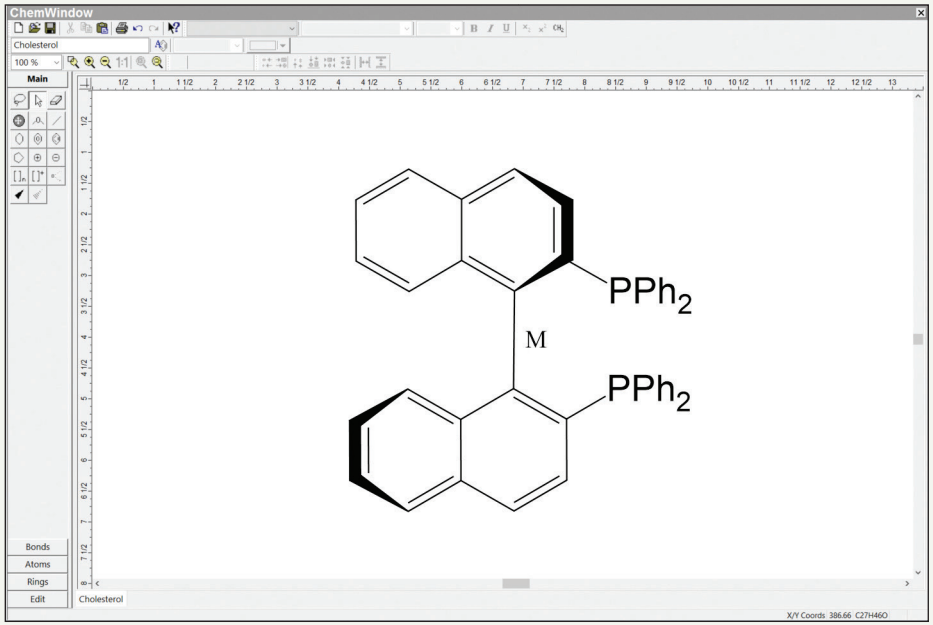
Explore the Tools In-Depth

- Basics Toolbox
- Data Toolbox
- Additional Tools

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 stereochemical 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

Advanced Stereochemical Recognition— Not Available in Other Packages!

Wiley's KnowItAll ChemWindow Edition includes technology to recognize stereochemistry not available in other structure drawing packages. Using this technology, KnowItAll is able to interpret structures (drawn or imported) using traditional stereochemical drawing conventions. KnowItAll's ability to understand and preserve the stereochemical intent of each structure is critical to building any database containing structures and relating records to one another when mining and searching the data.

Supported stereochemical descriptors include:

- Tetrahedral chirality centers (R/S), including spiro compounds
- Chirality axes such as those found in allenes and cumulenes with an even number of double bonds (M/P)
- Stereogenic axes such as found in some o-substituted biphenyls (M/P)
- Helical stereogenic axes (M/P)
- Chirality planes such as found in substituted cyclophanes (M/P)
- Pseudochiral (pseudoasymmetric) centers (r/s)
- Pseudochiral (pseudoasymmetric) centers (m/p)
- Cis/trans isomers as found for double bonds and cumulenes with an odd number of double bonds (Z/E or seqcis/seqtrans)
- Enantiomorphic cis/trans isomers as found for double bonds and cumulenes with an odd number of double bonds (seqcis/seqtrans)

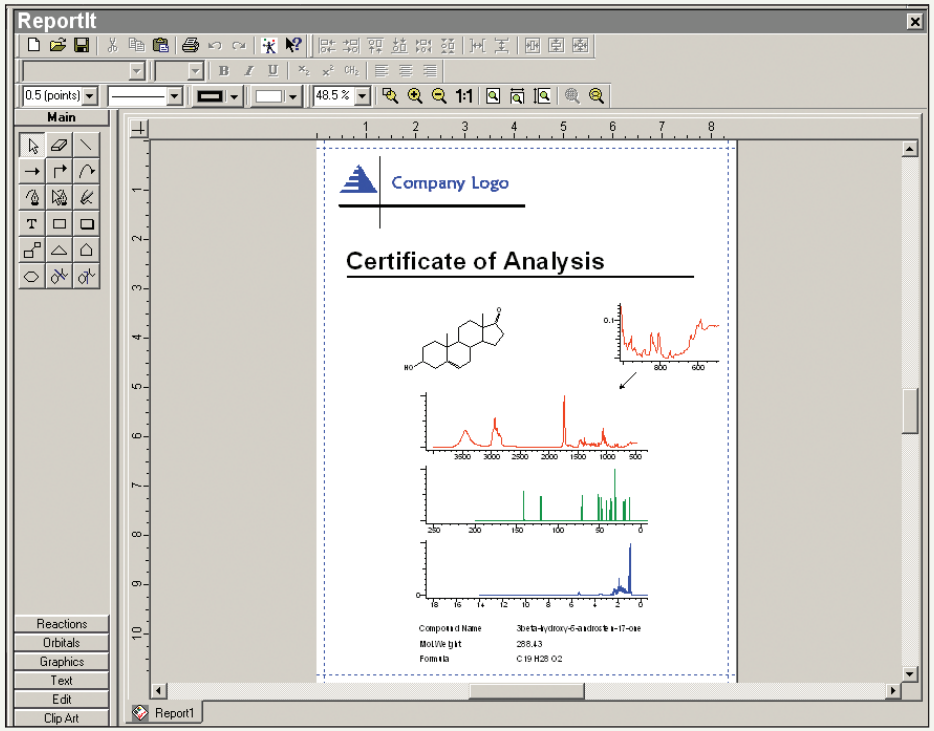
ReportIt™

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

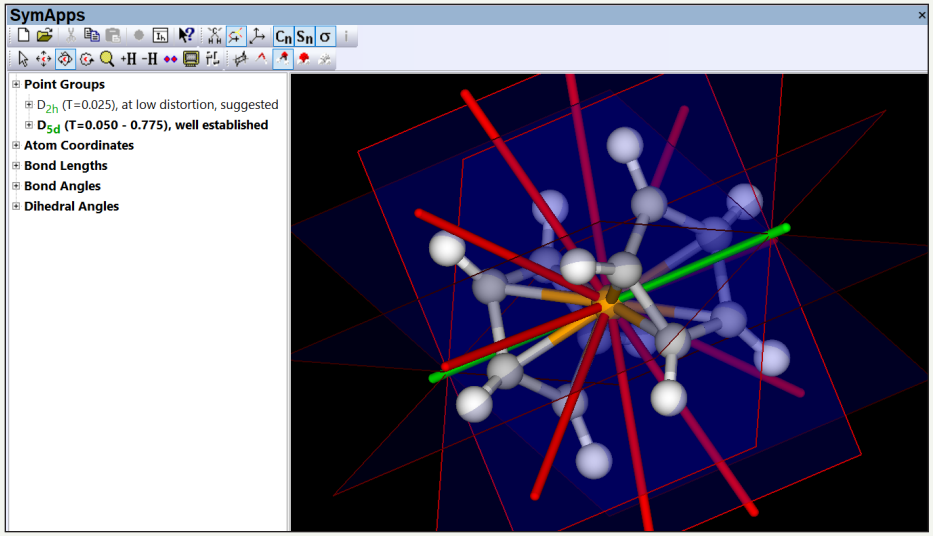


SymApps™

3D Presentations & 3D Modeling

SymApps is a professional symmetry analysis and 3D molecular rendering program, designed for desktop visualization and publishing. A modified MM2 force field minimization module converts 2D structure drawings to 3D in just seconds.

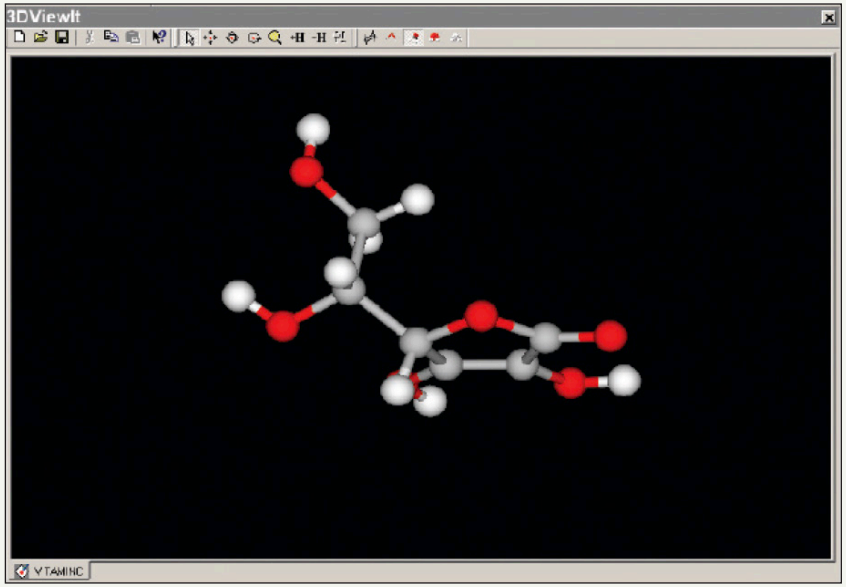
SymApps calculates, displays, and animates the symmetry for a molecule including rotation axis, mirror planes, and inversion centers. Create movies for three basic rotations and export them as .avi files that will run in any Windows application that supports this format. SymApps also allows calculation of point groups, bond lengths, angles, and dihedral angles for all atoms in the structure.



3DViewIt™

3D Structure Drawing

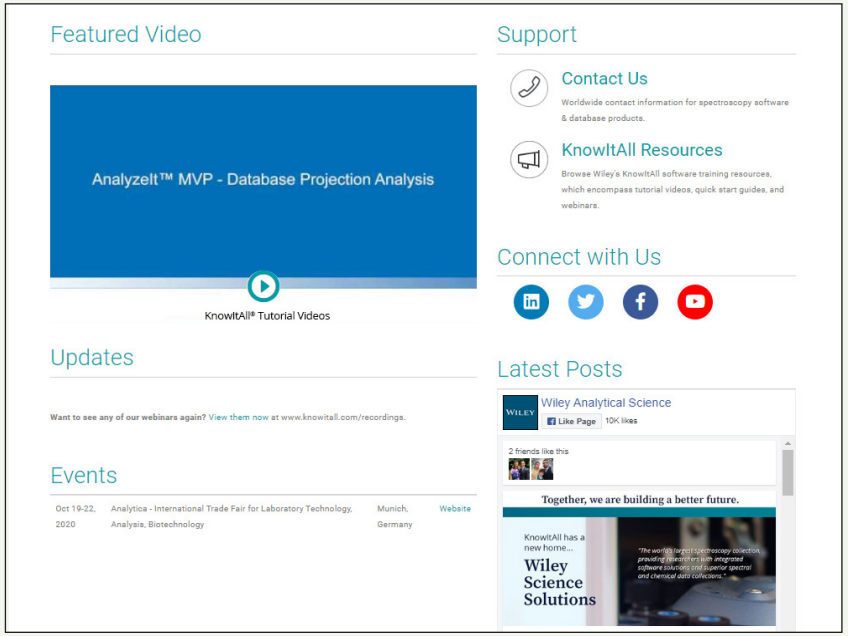
3D ViewIt allows the input of and visualization of 3D structures. A rudimentary 2D to 3D conversion is included for 2D structure files. The adjustable color display for atoms, bonds, and backgrounds provides high-quality, realistic 3D drawings, complete with spacefill, ball and stick, stick, and wireframe display options.



BrowseIt™

Web Training Resources

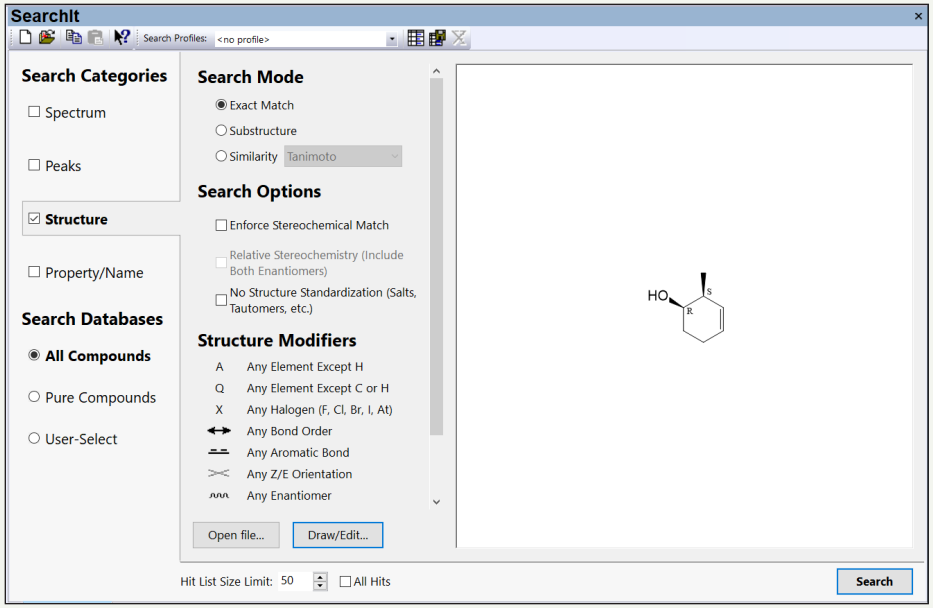
BrowseIt is a web browser built into the KnowItAll software with links to KnowItAll tutorial videos and other resources for KnowItAll users.



SearchIt™

Database Searching

SearchIt allows researchers to import data and search against user-generated as well as reference databases. Searches are fully customizable and are driven by powerful algorithms. Searches can be performed by name, structure, substructure, properties—in any combination.



MineIt™ / Database Building

Database Building, Mining, & Management

Researchers can build searchable databases of chemical structures and other relevant information, such as chemical properties.

Key Features

Build Databases

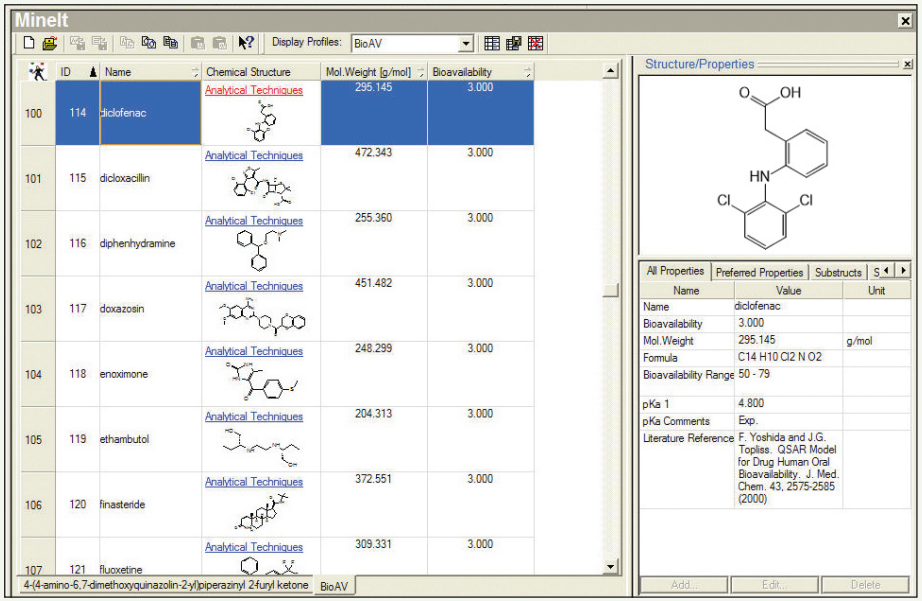
- Directly import structures drawn in ChemWindow into a database
- One-click import of existing structures from multiple structure formats with stereochemical bonds and identifiers (ChemDraw - *.cdx, CML - *.xml, Hampden - *.hsf, InChI - *.txt, JCAMP - *.dx, *.jdx, BIOVIA/MDL - *.mol, *.rxn, Smiles - *.smi, XYZ - *.xyz, etc. or *.csv format)
- Enhance each record with properties, such as boiling point, melting point, etc.
- 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)
- Quickly add properties and structures from PubChem to your database
- Use “Batch Import and Export” for efficient handling of structure and property files
- Make database more powerful by attaching spreadsheets, MSDS, and other documents or adding hyperlinks to web pages
- Categorize chemical structures of controlled substances according to Drug Enforcement Agency regulations (batch processing available)

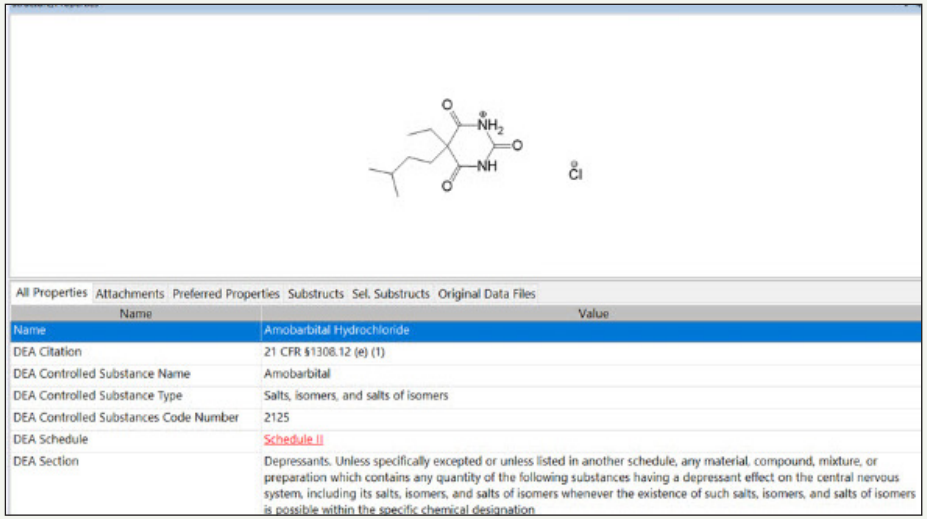
Customize Databases

- 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

Store and Search Complex Diastereomeric Mixtures

Create and search records representing complex mixtures of diastereomers Rather than adding multiple structures per record to specify all stereoisomers, KnowItAll’s unique color-coding system allows the user to specify centers with absolute stereochemistry and groups of two or more centers with the same relative stereochemistry. This results in an unprecedented system that easily and elegantly allows complex diastereomeric mixtures to be stored, searched, and retrieved from a database.



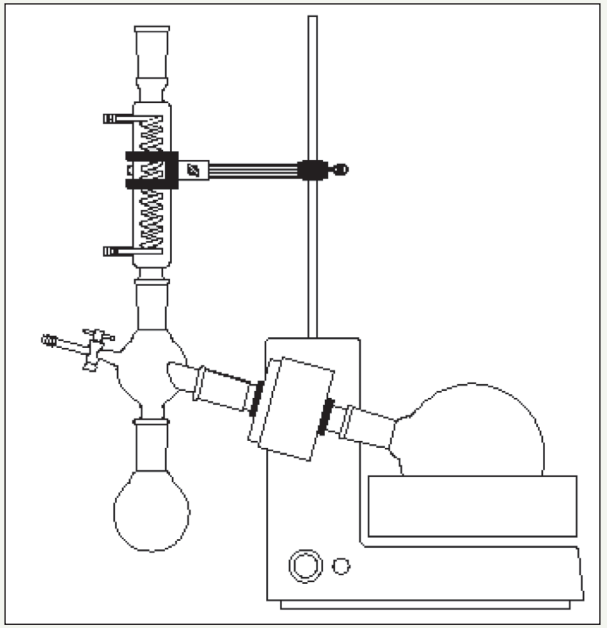


Clip Art Libraries (Included in ReportIt)

Clearly Illustrate Experiments and Engineering Processes

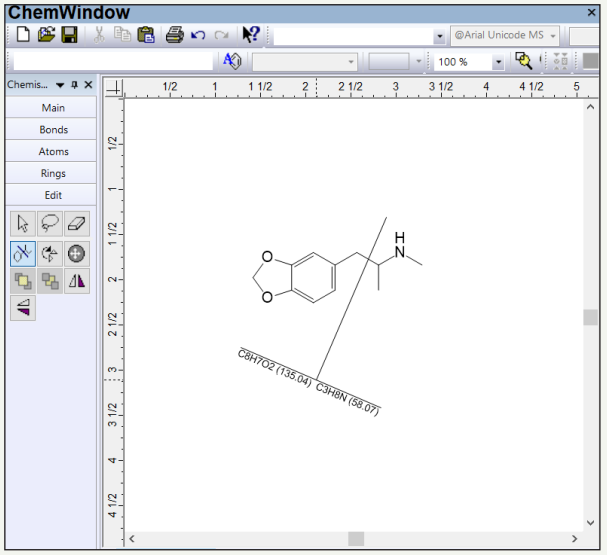
The Laboratory Glassware Collection contains more than 130 Illustrations to help communicate and document experiments. All pieces are drawn to scale and snap together at joints for easy construction.

The Chemical Engineering Collection offers over 250 process flow symbols to draw realistic process flow diagrams. Includes furnaces, filters, compressors, coolers, exchangers, evaporators, silos, separators, tanks, vessels, and valves.

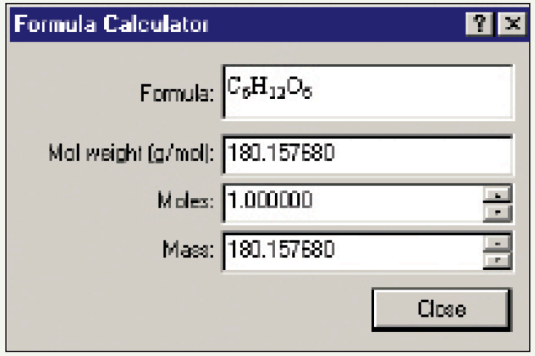


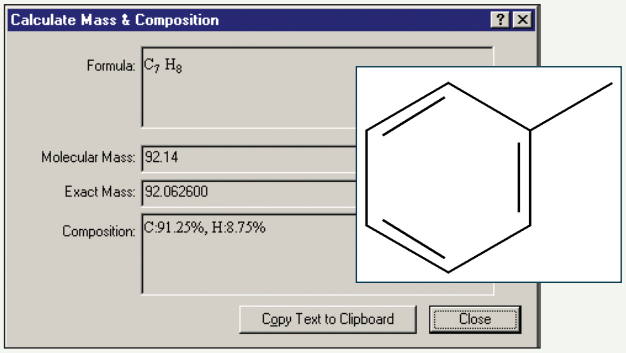
MS Fragmentation Tool (Included in ReportIt)

The MS Fragmentation Tool is the fastest way to determine whether a proposed structure matches the mass spectral data. This tool draws a movable fragmentation line through the proposed structure and displays the mass for the fragments on both sides of the line.



Calculation Tools (Included in ChemWindow)





Easy Mole-to-Mass Conversion

Calculate Mass from Structure

Plus NEW MS calculators for elemental composition and isotope distribution.

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sciencesolutions.wiley.com

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