Software for Structure Drawing, Data Management, & More

KnowItAll® ChemWindow® Edition
Draw Structures, Create Reports, & Manage Data

The award-winning KnowItAll Informatics System, ChemWindow® Edition offers complete, unified system to draw, modify, store, search, and retrieve chemical structures and other relevant information. Now researchers have all the data and software solutions they need in one place.

**Versatile Toolboxes.**
Draw structures, publish reports & more.

**True Integration.**
Instantly transfer data from one application to another.
The KnowitAll interface is designed so the user can transfer information from one tool to another, and move from one task to the next, without having to leave the main interface or open another program. Multiple tasks are performed using logically grouped "toolboxes." Because all the tools are located in a single, integrated environment, using this system will invariably save time and improve workflow. Ultimately, by combining tools and data into one system, the end result is greater ability to extract knowledge from data.

### Basics Toolbox

<table>
<thead>
<tr>
<th>Tool</th>
<th>Description</th>
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<tbody>
<tr>
<td>ChemWindow®</td>
<td>2D structure drawing (includes advanced stereochemical recognition not available in other packages)</td>
</tr>
<tr>
<td>ReportIt™</td>
<td>Publish professional reports, with structures and more</td>
</tr>
<tr>
<td>SymApps™</td>
<td>3D presentations and 3D modeling, plus calculation of point groups, bond lengths, angles, etc.</td>
</tr>
<tr>
<td>3DViewIt™</td>
<td>Visualization of 3D structures</td>
</tr>
<tr>
<td>BrowseIt™</td>
<td>Web portal with links to training resources and product news</td>
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### Data Toolbox

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<tr>
<td>SearchIt™</td>
<td>Database searching (search structures, properties)</td>
</tr>
<tr>
<td>MineIt™ / Database Building</td>
<td>Database display and mining; build databases with structures and properties</td>
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### Additional Features

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<td>Clip Art Libraries</td>
<td>Laboratory Glassware and Chemical Engineering collections</td>
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<td>Calculation Tools</td>
<td>Calculators for easy mole-to-mass conversion and calculation of mass from structure</td>
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<tr>
<td>MS Fragmentation Tool</td>
<td>Determine whether your proposed structure matches your mass spectral data</td>
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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, tools to calculate mass and formula, etc.
- 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
- Predefined styles for captions and structures

Advanced Stereochemical Recognition—Not Available in Other Packages!

Bio-Rad’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. It is compliant with the most recent IUPAC structure representation conventions as defined by the IUPAC Nomenclature of Organic Chemistry (Blue Book), 2013 Edition.

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)
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
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.
Basics Toolbox

3DViewIt™

3D Structure Viewing

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™ 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.
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
- Enhance each record with properties, such as boiling point, melting point, etc.
- Quickly add properties and structures from PubChem to your database
- Use “Batch Import and Export” for efficient handling of structure and property files
- “Auto-Property” computes values such as formula, molecular weight, etc. for entire datasets
- Make database more powerful by attaching spreadsheets, MSDS, and other documents or adding hyperlinks to web pages

Customize Databases
- Databases can be customized to meet laboratory specifications
- Users can create custom fields to support associated metadata 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.
Additional Software and Features

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)

Formula Calculator

<table>
<thead>
<tr>
<th>Formula</th>
<th>C₈H₁₃O₆</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular Weight (g/mol)</td>
<td>180.157630</td>
</tr>
<tr>
<td>Moles</td>
<td>1.0000000</td>
</tr>
<tr>
<td>Mass</td>
<td>180.157630</td>
</tr>
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Easy Mole-to-Mass Conversion

Calculate Mass from Structure