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:

• Structure Drawing & Reporting
• Chemical Information Management
• Data Searching & Analysis

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

Versatile Toolboxes.
Draw structures, publish reports & more.

How the Interface Works: 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.
What’s Is Included?

The KnowItAll ChemWindow Edition offers the following tools.

**Basics Toolbox**
- **ChemWindow**® 2D structure drawing (includes stereochemical recognition)
- **ReportIt**TM Publish professional reports with structures and more
- **3DViewIt**TM Visualization of 3D structures
- **SymApps**TM 3D presentations and 3D modeling, plus calculation of point groups, bond lengths, angles, etc.
- **BrowselIt**TM Web portal with links to training resources and product news

**Data Toolbox**
- **SearchIt**TM Database searching (search structures, properties)
- **MineIt**TM/Database Building Database display and mining; build databases with structures and chemical and physical property information

**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

See KnowItAll in action at www.training.knowitall.com
ChemWindow® provides an advanced set of drawing tools — just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

**Key Features:**
- Customizable toolbars with tools to draw chemical structures, including bonds, rings, atom labels, charges, etc.
- Chemical recognition features such as hot keys, chemical syntax checker, tools to calculate mass and formula, etc.
- Stereochemical recognition including R/S and E/Z isomers
- OLE (Object Linking and Embedding) technology for in-place editing in word processing and presentation software
- Predefined styles for captions and structures
- Compliant with the most recent 2008 IUPAC structure representation conventions

**Easily Import Existing Structures**
For customers using ChemDraw, files can be imported directly into ChemWindow. For those using ISIS/Draw, exported MOL files can also be imported. Many other file formats are also supported.

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**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.
- OLE (Object Linking and Embedding) technology for in-place editing in word processing and presentation software
- Advanced editing options to align, space, center graphics, and rotate captions
- Predefined styles for captions and structures
- 3D structure visualization for high-quality, realistic 3D drawings
- Table tool to enter and organize data
- Annotation tool to link objects like structures to text graphics or captions
- Spectrum/chromatogram Import in common native file formats
- Multi-spectrum displays including three display modes: overlay, stack, and offset
- Advanced spectrum display editing features to customize the appearance of spectra and chromatograms, including axes, colors, labels, etc.
3D Structure Viewing

3DViewIt 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.

Web Training Resources

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

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.
SearchIt™ allows researchers to import 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.

Database Building, Mining, & Management
Researchers can build searchable databases of chemical structures and other relevant information, such as chemical properties. Import structures in MOL and SDF file formats to create databases quickly from existing data.

Customize Databases
Create customized fields or “preferred property” forms so users can enter properties in a consistent way and thus maintain the integrity of data throughout the organization. There is also the option to password protect data and manage access privileges.

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.

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

New Feature! Quickly add properties & structures from PubChem to your database.
Additional Software & Features

Clear Illustrations of 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, towers, 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 DrawIt)

**Formula Calculator**

```
Formula: C6H12O6
Mol weight (g/mol): 180.157630
Moles: 1.000000
Mass: 180.157630
```

**Easy Mole-to-Mass Conversion**

**Calculate Mass & Composition**

```
Formula: C6
Molecular Mass: 76.14
Exact Mass: 76.063600
Composition: 58.9239%, 41.0761%
```

**Calculate Mass from Structure**