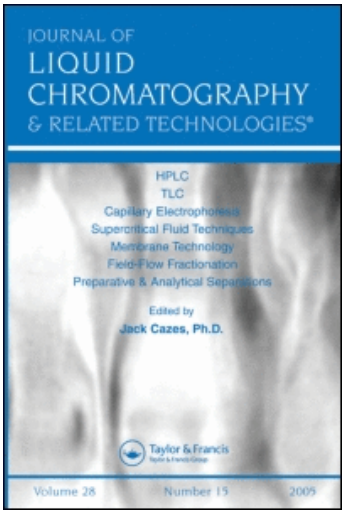

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Software Review

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SOFTWARE REVIEW

ChemWindow CHEMISTRY DRAWING SOFTWARE, Version 2.0.1, SoftShell International, Ltd., 715 Horizon Drive, Suite 390, Grand Junction, CO 81506, USA, 1992, $499.00.

ChemWindow is a software package for drawing typeset-quality molecular structures. Numerous features have been included to make this task a simple one. The software permits output of molecular graphics to formats that are compatible with all Windows applications, with WordPerfect (as .WPG files) and with many other DOS applications. A built-in palette of work tools is used to easily select functions needed to draw specific structural features, e.g., Bezier curves and arrows; multiple, unlimited bond attachments to atomic character labels, scaling f structures; multiple fonts for atoms, labels and captions, even with kerning. The ability to use multiple "undo" commands to sequentially backtrack to remove unwanted changes make ChemWindow very forgiving and unintimidating to the novice and occasional user. A particularly nice feature is the use of a "Join" command; with it fused ring systems may be readily assembled by simply bringing individual rings elements near each other, then selecting "join" from the menu.

The SoftShell Structure Album contains hundreds of useful structures to use as starting points to draw other structures. Included in the album are amines; acetylcholine-related compounds; alkaloids; amino acids; AMP, CMP, GMP & UMP; amphetamines; antibiotics; artificial sweeteners; ATP, ADP; cephalosporins; chlorophyll; disaccharides; DNA; hallucinogens; hematin; hexoses; hormones; nucleic acids; opiates; penicillins; pentoses; pollutants; porphyrins; basic rings and fused rings; arenes, heterocyclics; tricyclic antidepressants; vitamins.

Installation is straightforward. Windows 3.0 with Adobe Type Manager or Windows 3.1 alone is required. The program is menu-driven and easy to learn. With only the menus and the tool palette one can immediately start creating relatively complex structures. The well-written manual takes you through the use of the drawing tools in a step-by-step fashion, with illustrative examples to try out. Now, let's look at some of the available tools.

A **Selection Tool** is provided to manipulate objects, to "select" (identify) objects upon which a subsequent command will operate, change line thickness, identify fonts, etc. With it, objects may be moved, scaled, stretched and duplicated. This last feature is particularly useful when a reaction sequence is to be drawn.

Parts of structures may be selected with the **Lasso Tool** to be moved, stretched, copied, cut, duplicated, sent behind or in front of other elements without affecting the rest of the structure. Thus, for example, a six-membered ring may be bent to a chair or boat form by "**lassoin**g the appropriate atoms in the ring.

An **Acyclic Chain Tool** may be used to draw chains with, or without, alternating double bonds, in any direction (any angle). As each "link" is drawn, the software displays a count of connecting bonds. The "up/down" orientation of the chain may be easily changed.

Atomic labels are automatically subscripted and superscripted with the **Label Tool** when "Formula" style is enabled. Atomic labels are either entered as replacements for unlabelled atoms (mouse click) or as substituents at the end of a bond (mouse drag). To insert an atom on a ring, at the juncture of two bonds (as in heterocyclics) the label is entered, then the "hit" box at the juncture is highlighted and the mouse is clicked. That's all there is to it! Character spacing (kerning) is adjustable.

Bond arrow and ring lengths are selected within a Style dialog box. The angle of bond placement is selected in a second ("Next") Style dialog box.

The **Bezier Curve Tool** is used to draw a curved line smoothly in any direction or angle. This tool is useful for showing bond and electron movement, to draw curved bonds and to label bond angles. Curved arrows are also useful as pointers to draw a reader's attention to a specific element of a structure or reaction sequence. Line thickness and the size of arrowheads are adjustable.

The **Bond Tools** include drawing capabilities for standard (straight) bonds, dashed bonds, hashed (shaded) and solid wedge-shaped bonds, bold bonds, wavy bonds and curved bonds (using the Bezier Curve Tool). Thus, stereochemical features of molecules may be readily illustrated.

Ten **Ring Tools** provide shortcuts to drawing cyclic structures of various sizes and shapes, including chair and boat forms of six-membered rings (cyclohexanes, saccharides, for example). The Benzene Ring Tool offers the option of standard or Kekulé format. Unsaturation may be added, and line widths, size and other ring settings can be selected.

Several kinds of arrows may be selected and drawn with four **Arrow Tools**. Reaction (single head), resonance (doubled head), equilibrium (double arrow) and dashed arrows are available.

The **Template Tool** and the **Album Tool** are used to store graphics and to select pre-drawn, previously saved molecular structures. Templates are molecular skeletons not yet containing labels. Similar to Ring Tools, structures may be rotated, sized and fused in the work area. You can bring together your most-used templates in the Template Tool for use later on. The same structure will never have to be drawn twice!

The Album Tool is a scrapbook for storing molecular graphics and other chemistry drawings. Any graphic that can be pasted into ChemWindow may be stored in an Album. This includes paint graphics, bitmaps, PICT files, clip art and other compatible file formats.

Additional tools include a **Drawing Tool** (for drawing boxes, brackets, orbitals, Lewis dots, circled charges, etc.), two **Arc Tools** (to draw circles, ovals, arcs and curved arrows with one- and two-electron arrow heads) and an **Eraser Tool** for removing unwanted parts of structures. The eraser tool is particularly useful for modifying structures from the Template and Album files.

Several Icons perform such functions as obtaining a mirror image of a structure in the work area (Flip Icon), rotating a structure (Freehand Rotation Icon), grouping multiple structural elements together (Group Icon), joining objects that were drawn separately (Join Icon). An Align Icon is useful for vertically and/or horizontally lining up unconnected pieces of large structures. An Align dialog box is used to specify the alignment mode.

An extensive context-sensitive help function is included in ChemWindow that answered most of the questions this reviewer encountered while drawing structures, using all of the available palette tools. Further competent assistance was provided by SoftShell's friendly technical service personnel.

Included with the ChemWindow package is a program called Molecular Mass Calculator, which calculates molecular mass, or "exact" mass used in mass spectrometry, from an empirical formula; isotopes may be marked and included in the calculation. Percent composition (by mass) may also be calculated.

ChemWindow is highly recommended for anyone who needs to draw molecular structures for preparing seminar slides, for inclusion in publications and for teaching aids. The user-friendly interface (pull-down menus and palette tools) makes this program easy to use. Even the occasional user, who may have a tendency to forget the "inner workings" of a software package, will have no trouble using ChemWindow. Its extensive capabilities for drawing all kinds of structural elements and structures make it the program of choice for the novice and professional alike.

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