ChemWindow, Version 2.11

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ChemWindow[1] is a Windows[2]-based molecular drawing program that is closely related to the Macintosh program ChemIntosh and a PC entry level program ChemWindow Classic. I found this program to be so powerful and easy to use that during the course of the review I deleted the drawing package I had previously used from my hard disk. This program is *fun* to use and produces a very high quality product. The authors have made a successful effort to accommodate the user with a program that has a very smooth operation and is easy to learn. I tested the program on a 386-33 clone *without* a coprocessor, a Gateway 486-33 system, and a 486-33 clone with a local bus. There is no question that, in common with many Windows programs, faster is distinctly better; however, even the 386 system was adequate. The main limitation occurred during drag operations to move or resize a large structure.

The interface for ChemWindow is easily accommodated by users familiar with the Windows environment and drawing tool icon palette/command menu approach that is common to most drawing programs. The point, click, and drag techniques common to many Windows programs are all used in an easily mastered way. The manual, which contains instruction for both ChemWindow and ChemIntosh, is well written and has an adequate index. Users familiar with other drawing programs can use the *Quick Start* section; however, the four short *Tutorial* exercises supplied take less than an hour and teach you the basic skills required in a logical and entertaining fashion. Beyond the initial tutorial sections, the *Reference Manual* section discusses the individual drawing tools and menu commands in detail. An extensive on-line Help system is incorporated into the program. Registered users receive a periodic newsletter and have access to user support via telephone, fax, and a bulletin board (BBS). The program comes with an album of structures which can be used as the starting point for new drawings and a freeware utility (SoftShell Molecular Mass Calculator) for calculating molecular weights and percent composition. Users that purchase version 2.11 will receive a free upgrade to version 3 when it is available. Network licenses are available with an academic discount if students use the network copies.

The construction of drawings is accomplished by a combination of commands from eight drop-down menus and thirty-nine drawing tools from the palette. Several of the common commands have keyboard equivalents (largely intuitive and easily remembered, e.g. Ctrl-A to select all the elements on the screen and Ctrl-C to copy selected items to the Clipboard for transfer to a document). There is some redundancy between the functions of the *Command Menus* and *Drawing Tools* (e.g. vertical or horizontal flipping of a selection) which increases the versatility of the package. Many of the Drawing Tools have enhanced capabilities when used in combination with the Shift, Alternate, or Control keys. For example, using a bond drawing tool alone produces a standard length bond, and using the tool with Shift key depressed relaxes the length constraint. As noted below, an on-screen prompt for the key enhancements is available when the Help Pane (see below) is active.

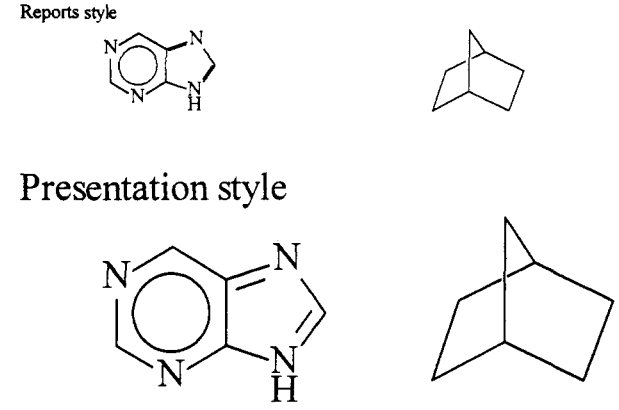

Figure 1. ChemWindow's drawing style.

Of the Command menus, three (Font, Size, Style) refer to the atomic labels and text captions. Only scalable fonts such as ATM or TrueType fonts are supported. If you are not using Windows version 3.1, Adobe Type Manager[3] and appropriate ATM fonts are required to make Greek letters and math symbols available; however, this is unlikely to be a problem since most users will have upgraded to the current version of Windows. *Captions* are typed directly in the drawing area using the *Text Tool*. Atom labels or summed formula elements (e.g. CH_3CH_2) are entered by placing the cursor into an area at the top of the active window called the *Label Pane*. In this area numbers without charges are assumed to be subscripts and signed numbers superscripts in accordance with most chemical applications. The contents of the *Label Pane* are then placed into the structure with the *Label Tool*. A superscripted atom label, e.g. ^{31}P, can be produced by highlighting the subscript number and using the *Style Menu* command for superscripting twice. This is an example of an operation that is best done by using the keyboard commands (Ctrl-Y for superscript and Ctrl-L for subscripts). This all sounds more complicated than it really is in practice. The *Formula Style* which automatically treats numbers as in the *Label Pane* can be turned on when *Text Tool* is being used.

The *Options* menu allows the choice between drawing *Styles* which control the default values for standard bond lengths, font sizes, etc. Two drawing styles, *Report* and *Presentation*, are predefined. The latter, involving bold lines and labels, etc., produces a drawing approximately two times larger than the *Reports Style* and is appropriate for the preparation of slides and figures. Figure 1 indicates the difference between these two drawing styles. The default values for bond lengths, widths, and text formatting for both choices can be modified by the user. Additional styles can be defined and saved as needed. Other choices in this menu involve toggle commands for the placement of the Tool Palette, to position vertical and horizontal rulers that report the cursor position at the top and left of the drawing area, and for the insertion/deletion of a reduced size view of the entire drawing in the upper right-hand corner of the drawing area. This latter is a very handy

feature since only 22% of the active drawing area can be viewed at a time. The *Arrange* menu controls grouping and ungrouping of components of a complex drawing to allow movement of several components together as a unit. Alignment and orientation of the components of a drawing are also addressed in this menu, as well as the choice to introduce a "break" in a bond line to denote which of two crossed bonds is closer to the viewer. The remaining menus, *File* and *Edit*, contain the file handling and cut/paste operations common to most Windows software and a powerful *Undo/Redo* option with a buffer that can hold several levels of drawing commands. A strong feature of the program are the *Load Album* and *Load Template* commands of the File menu. These commands allow any ChemWindow. CW2 file to serve as the basis for a new drawing through the *Album* and *Template Tools*. These powerful tools will be discussed further below.

Only a limited view of the power of this program can be presented here. The thirty-nine drawing tools of the *Tool Palette* allow placement of drawing elements by the click-and-drag procedure and involve ten ring types (n = 3–8, benzene, and six-member chair and boat) and seven different bonds. After initial placement, rings can be rotated around prechosen pivot bonds and atoms until the mouse button is released. Bonds are drawn at the default length and can be moved through a constrained set of angles relative to the point of attachment (15° steps). As noted above, many of the drawing tools are enhanced by pressing a key during the drawing operation. For the various bond tools, the Shift key relaxes the length constraint and the Control key the angle constraint in the placement of a new bond. Once placed, each element of a drawing can be moved or rotated freely, either individually, or when, *Grouped* as a unit.

There are several examples of refinements developed by the authors to make the program both powerful and easy to use. For example, using the *Selection Tool* to choose a drawing component allows the resizing of that element by the usual method of dragging on one of the drawing handles that appears on the screen. ChemWindow gives the user the advantage of a *dynamic-on screen display of the percent change in size* during the resizing operation. In a similar way, during a free rotation operation about a corner handle, *the current value of the rotation angle is displaced dynamically*. The same drawing handles can be used to "tip" a ring to produce an "edge-on-view". The *Lasso Tool* can be used to move a subset of the atoms of a ring, e.g. to convert a boat form of a ring to the twist boat. The *Acyclic Chain Tool* places a number on the screen during the drawing operation to indicate the current number of bonds in the chain. Each of these refinements makes a good program even better.

The remaining drawing tools include five styles of arrows, including curved, double-handed, and equilibrium arrows. Circles, ellipses, and arcs are available in both full and dashed formats. A *Bezier Curve Tool* is available for electron pushing diagrams or for calling attention to specific areas on a complex drawing. Several editing features, e.g. an "eraser", and tools to allow vertical or horizontal flips are available on the palette. Tools that parallel the alignment and grouping commands are included, a further example of the effort the authors have made to make this program powerful and user friendly.

Perhaps the three most powerful drawing tools are the *Album*, *Template*, and *Drawing Tools*. Selecting the third of these offers a choice of chemically useful "objects" and symbols, e.g. orbital surface diagrams, brackets, and "text boxes". The *Album Tool* can be "loaded" with any ChemWindow drawing and any of the "ungrouped" subunits of the file incorporated into a new drawing. Once a file is loaded into the album, a click on the album icon drops a menu showing the various components. Dragging the highlight over the desired unit selects that component, and placing it into the drawing area involves the usual "click–drag" procedure. Clear directions for constructing files containing frequently used subunits are given in the manual. The operation of the *Template Tool* is similar; however, any labels that are part of the drawing are ignored (apparently "circles or ellipses" designating conjugation are treated as labels). Therefore, choosing pyridine from a file loaded as a template inserts a six-member ring in the drawing area. Examples of drawing from the *Structure Album* and elements from the *Drawing Tool* are shown in Figure 2.

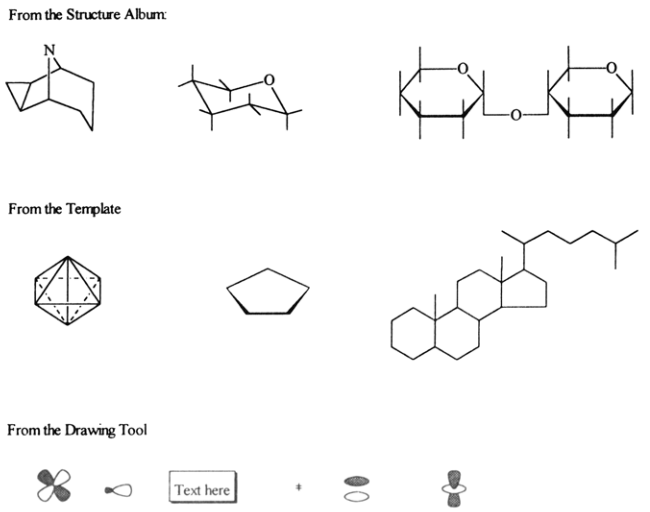

Figure 2. ChemWindow's "canned" structures.

Three *Help* elements are incorporated into the program. Clicking on the *Help Pane* option in the Help menu adds a context-sensitive help message directly above the drawing area. When you choose a drawing tool and move the cursor into the drawing area, brief reminders of the operation of the tool and any key press enhancements are displayed in the help pane. Choosing the *Help Window* places a side-by-side context-sensitive help window next to a reduced size drawing window with greater detail about the use of the active tool. Finally, *Help Topics* displays a set of brief essays on aspects of the operation of the program. These are *not* the equivalent of an on-line Reference Manual; they are brief and oriented toward very specific questions such as file import/export. A particular help topic *Troubleshooting* deals with problems observed with specific software packages and work-around procedures for programs that do not accommodate the .WMF format.

The program will print structures via Windows Print Manager; however, most users will want to incorporate structures into word processing or other software. Several file transfer methods are available, with the simplest being to copy the drawing to the Clipboard and paste it into the document in question. Drawings can be returned to ChemWindow via the clipboard for editing. I tested the file transfer procedure with Word for Windows,[4] and it worked without problems. The special on-line help topic noted above describes work around procedures for transferring drawings to specific applications, e.g. PC Paintbrush, that do not support the .SCF and .WMF formats used by the program for most file transfers. In addition to these two export formats, ChemWindow will export files in the .EPS, .WPG (WordPerfect), and Molfile formats. The latter can be used to export drawings to programs such as REACCS.[5] Import file formats that are supported

are .SCF, .WMF, ChemDraw 2.*x*, Molfile, and earlier versions of ChemWindow. A clear discussion of the use of the various file formats is given, including any disadvantages such as the loss of the ability to edit drawings in some cases. To incorporate additional graphic elements from another program, e.g. spectra, they must be in the form of *placeable.WMF* format. The user support suggests using the HiJaak[6] program to accomplish this task. Increased flexibility in file import is promised for the next major upgrade in ChemWindow (version 3).

In summary, ChemWindow is a powerful and easy to use molecular drawing program, easily the best of three or four I have used. The current version is a delight to use, and the proposed changes suggested for version 3 will make it even better. SoftShell International has announced a free upgrade to that version for purchasers of version 2.11, so there is no reason to wait. My contacts with the support personnel at SoftShell have been very cordial and helpful (e.g. they replaced a defective installation disk by priority mail and hand checked it before shipping). Several colleagues have verified that user support is a strong feature of this company. The possibility of file sharing with ChemIntosh may be helpful in some environments. I would encourage anyone in the market for a molecular drawing program for use in the Windows environment to seriously consider ChemWindow.

REFERENCES AND NOTES

(1) ChemWindow, Version 2.11, SoftShell International, Ltd., 715 Horizon Dr., Suite 390, Grand Junction, CO 81506. Telephone: 303-242-7502. Fax: 303-242-6469.
(2) Windows, Version 3.1, Microsoft Corp.; One Microsoft Way, Redmond, WA 98052-6399.
(3) Adobe Type Manager, Adobe Systems Inc., P. O. Box 7900, Mountain View, CA 94039-9880.
(4) Word for Windows, Version 2.0C, Microsoft Corp., One Microsoft Way, Redmond, WA 98052-6399.
(5) REACCS, Molecular Design Ltd., 2132 Farallon Dr., San Leandro, CA 94577.
(6) HiJaak, Inset Systems, Inc., 71 Commerce Dr., Brookfield, CT 06804-3405.