ISIS/Draw for the Macintosh[1,2]

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CONFIGURATION

I installed ISIS/Draw v.1.0 on a Macintosh SE/30 with 2 MB RAM and a 40-MB hard disk. The recommended hardware platforms for ISIS/Draw are

- Macintosh IIcx, IIx, IIci, IIsi, or IIfx (68030 microprocessor)
- 2 MB RAM
- AppleColor monitor
- PostScript printer
- Adobe Type Manager
- 80 MB hard disk

In addition, the following are required

- Version 6.0.5, 6.0.6, or 6.0.7 system software
- mouse
- 1.5 MB of free hard disk space

As my Macintosh had an earlier version of the operating system, I first had to upgrade to System 7.0 before I could run the software (ISIS/Draw was clever enough to prevent me from running it before the system upgrade). System 7.0 is a huge improvement over previous versions of the Macintosh operating system (e.g., it gave the possibility of using part of my hard disk for virtual memory, turning my Mac into a virtual 4-MB machine). It is a pity that ISIS/Draw does not yet support some of the nice features of System 7.0 such as 'balloon help'.

OVERALL IMPRESSION

ISIS/Draw is the "Rolls Royce" of chemical structure drawing programs. In fact, the first thing to understand about ISIS/Draw is that it is more than a chemical structure editor—it also serves as the front end of the whole ISIS distributed system. As I only had access to ISIS/Draw, I was not able to explore its relationship to ISIS/Base and its ability to access both local and remote chemical structure databases. I will therefore limit my comments to those aspects of ISIS/Draw relevant to its use as a chemical structure editor. The dual functionality of ISIS/Draw does lead sometimes to an apparent complexity of the program which other chemical structure editors do not have.

To further complicate this review, it is important to recognize that ISIS/Draw is really two programs in one: a chemical structure editor (comparable to ChemDraw or ChemIntosh) and a general sketching program for preparation of presentation graphics (comparable to say, MacDraw). Chemical structures prepared using the chemical structure editor may easily be integrated into sketches but the reverse is not true.

The documentation is excellent, and I enjoyed using the tutorial manual to learn the basic features of the software. In addition to the tutorial, the documentation consists of an installation and orientation guide, a reference manual, and a quick reference booklet. There is also an extensive on-line system which is extremely comprehensive but a little daunting. The help index consists of some 92 screens-full of information on my Mac, and even the table of contents occupies 17 screens!

CHEMICAL STRUCTURE EDITOR FEATURES

Molecular Design Limited (MDL) has carefully followed the Apple Human Interface Guidelines and has developed a software package which has the look and feel of a Macintosh software product. There are a number of pull-down menus: file, edit, options, object, style, templates, and chem, each of which provide access to a comprehensive set of commands. On the left of the screen arranged in a vertical palette there are a number of molecule tools: select, select/rotate, component, eraser, text, atom, single bond, double bond, triple bond, wedge up bond, wedge down bond, either bond, rectangular up bond, and regular down bond tools. A horizontal palette below the menu bar allows the user to select molecule or sketch mode and, in molecule mode, provides some common ring system template tools.

The structure editor offers many alternative ways of performing simple functions (e.g., there are six ways to select objects), and the user is advised to adopt preferred methods of his/her own to achieve the most simple tasks or go insane!

ISIS/Draw has clearly benefitted from the recent advances in the design of user interfaces for chemical structure editors made by its competitors. However, there are many innovations, and I particularly liked the way in which rings can be sprouted off other rings (MDL has made the assumption that biphenyl-type ring systems are more common than spiro-fused ring systems). I also liked the way in which the user can choose the point of attachment when using templates.

I missed the lasso tool and the multiple level undo facility found in the STN Express chemical structure editor (among others). I disliked the multiple use of cursor types (e.g., the cross-hair cursor) as I sometimes became confused about which tool I was using. I found the multiple level menu for labeling the less common elements, tiresome and complex. I hope MDL will improve this in a future version of the product.

There are many features in the chemical structure editor which have little relevance to the task of producing publication quality diagrams (e.g., although I liked the atom lists, I cannot imagine wanting to use them in a structure diagram). It is a pity that some way could not have been found of hiding this level of complexity.

SKETCH FEATURES

In the sketch mode, the vertical palette changes and a series of drawing tools are available: select, rotate/resize, eraser, text, brackets, square box, rounded box, line, polygon, ellipse, arc, and continuous line tools. A font manager is available from the style menu; I created the sketch described in the tutorial manual but did not have time to explore this mode further. I particularly liked the alignment capabilities of the program and used them to align objects to vertical and