TECHSIGHTING
SOFTWARE

Equationsmith

Equations, text, and graphics must often be combined when creating scientific presentations. This can be a time-consuming and tedious process. Most equation editing software packages cannot easily deal with graphics, and many graphics programs lack efficient text editing capabilities for equation input. Equation Illustrator V addresses these issues by integrating solid text editing capabilities with a simple illustration package.

Equation Illustrator V
MGC Software
Altrincham, Cheshire, UK
$20
www.mgcsoft.com

Equations are constructed in Equation Illustrator V by selecting symbols from an extensive set of palettes. Additional symbols are available by choosing different font sets from a drop-down menu bar. Clicking a palette symbol places the character at the cursor insertion point.

The Equation Illustrator V text editor really shines in its easy-to-use text layout controls. Three buttons control the movement of a character in increments of one pixel. Two additional buttons allow one click to change the font size. Once an expression is completed, it can be placed on the page either with text layout controls (tab, space, return), or it can be converted into a graphic by selecting a region and using the "convert to picture" option. These graphical elements may be moved by clicking and dragging.

Although the drawing function of Equation Illustrator is similar to simple drawing applications such as Microsoft Paint, the features are slightly different. For example, shapes are selected from a drop-down menu. Clicking at any point on the layout area places the shape at that point. Placement requires some forethought because it is not possible to move shapes with a click and drag operation. Rather, position is controlled by entering the *x*-*y* position in pixels into a dialog box. It is also possible to convert the shape to a graphical element, but the tool only selects squares, so placing the shape too near other elements results in a picture with bits of other elements included.

A useful feature is the "wave" option in the shapes drop-down menu, which permits precise control of the period, wave height, and start angle of a full sine wave or negative and positive half-waves. The rise, fall, and pulse width of a square wave can also be controlled.

The Equation Editor produces bitmapped images, which yield coarse print-preview images missing some elements, although the final printed output is not affected. All fonts, symbols, and pictures are properly smoothed. Output formats include Enhanced Metafiles, JPEGs, bitmaps, and GIFs.

An extensive online manual is included in the package, and technical support is provided for registered users. The next version of the program, currently in development, includes the ability to move shapes and more extensive drawing controls. For the small purchase price, Equation Illustrator offers an excellent mix of features.

—ERIC BASHAM

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TECHSIGHTING
SOFTWARE

Infrared Spectra Vending Machine

HaveItAll IR is a product for Windows 95, 98, NT, or 2000 that offers a revolutionary way to access the world's largest collection of infrared (IR) spectra. In contrast to Web- or server-based spectral databases, HaveItAll IR provides over 200,000 spectra on a single CD-ROM disk. All spectra are available to view and search as often as one needs, but the customer pays only when wishing to examine the record for a compound (or class of compounds) that matches their search criteria. This is accomplished with an electronic Hit List Key, purchased separately.

HaveItAll IR
Bio-Rad Laboratories, Sadtler Division
Philadelphia, PA
$1750
888-524-6723
www.sadtler.com

The HaveItAll IR package (database and search software) occupies 354 MB of hard disk space. It contains 89 different libraries covering a broad range of compounds in categories that include polymers and related compounds, pure organic compounds, inorganic compounds, and organometallics. Also included are over 3300 Raman spectra. The basic package contains a Look-Up function with a one-year license.

HaveItAll IR's Look-Up License allows one to look up compounds in the HaveItAll IR databases using name or structures as criteria to retrieve reference spectra. The annual Look-Up License allows one to perform as many look ups of names or structures as desired during the time of the license and does not require the use of a Hit List Key.

HaveItAll IR's spectrum searches include full and limited range spectrum searches, peak searches, and property searches. This powerful function allows one to identify or classify unknown spectra by comparison to spectra in the hit list. HaveItAll IR can read spectra in 18 file formats. In contrast to name and structure searches, spectrum searches return potential matching spectra (up to 50), but the spectra are not, as a default, linked to names or structures. To obtain the record(s) about the compound(s) found in a spectrum search, a prepaid electronic Hit List Key must be used to unlock and view all the pertinent information for the compounds in the list.

HaveItAll IR's searches are fairly rapid. A simple structure-based search of a single molecule (octanol) took less than two minutes on a first generation Pentium 233 MHz PC with 64 MB of RAM. Although one can search all or some of the databases in any of the 89 different libraries, It would be more useful to be able to choose categories or classes of compounds instead.

HaveItAll IR provides a simple structure builder called Query Editor, which looks like a trimmed-down version of Bio-Rad's ChemWindow product (*1*). The Query Editor's somewhat limited functions allow the user to import only ChemWindow formatted files and permit export only via the clipboard. One cannot save a structure file, so when another search is carried out it must be redrawn.

HaveItAll IR's new mechanism for spectroscopic database distribution will be welcomed by both industrial and academic professionals. The Look-Up feature is cost-effective and saves time. Industrial users, in particular, will like accessing the large database of IR spectra in-house without having to upload potentially proprietary information to a Web site for searching.

—SATYAM PRIYADARSHY AND ASHVANI K. SINGH

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Reference

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