TECHVIEW
SOFTWARE

Dry Chemistry

Brian Shmaefsky

Sadtler Suite is a software package for drawing chemical structures and then analyzing them. It is composed of four software products: ChemWindow, IR SearchMaster, IR Mentor Pro, and SymApps. ChemWindow designs chemical structures and performs several analyses. IR SearchMaster analyzes structures and imports information stored in databases of infrared (IR) spectra. IR Mentor is a database of structures useful for comparing simple or complex spectral information (Fig. 1). SymApps is a companion tool for rendering three-dimensional (3D) chemical structures.

Accompanying Sadtler Suite are separate, comprehensive manuals for ChemWindow, IR SearchMaster, SymApps, and the supplementary software, IR Mentor Pro. All of the guides have step-by-step instructions for using the software, and each contains a glossary of terms and a comprehensive index. In addition, IR Mentor Pro includes a tutorial on how to obtain and analyze IR spectrum data. The Sadtler Division of Bio-Rad offers e-mail support for ChemWindow, IR SearchMaster, and IR Mentor Pro. Online support and animated tutorials are available (www.bio-rad.com).

Sadtler Suite
Bio-Rad Laboratories, Sadtler Division.
Philadelphia, PA.
$2,000,
$1,500 (academic).
1-888-5-BIO-RAD.
www.bio-rad.com/73650.html

ChemWindow provides sophisticated chemical drawing functions and predicts ^{13}C nuclear magnetic resonance (NMR) shifts, mass spectral results, and IR spectra of chemical structures. ChemWindow has a work toolbar and blank page window very similar to those in word processors. This window is called the "paper" and serves as a sheet of drawing paper for designing structures. It also acts as a pasteboard for placing spectra and chromatograms. The toolbar of ChemWindow is set up so the user can perform the basic drawing and analytical functions by clicking on icons, and it can be customized to increase or decrease the number of icons, as desired.

The functions for drawing chemical structures in ChemWindow are elaborate. The program can be used to produce publication-quality structural drawings in both black-line and color. Figures can be sized appropriately for both publication and presentation needs. Structures are simply constructed by dragging and clicking atoms, bonds, functional groups, and rings from the toolbar icons. The different structural components snap together along a grid, making it easy to construct complex molecules. Complicated molecular constructions are simplified by chemical structure templates that can be added to the toolbar.

The drag-and-click feature also allows simple structures to be converted into cyclic compounds. Aromatic templates can be modified by substituting atoms and adding functional groups. In addition, the toolbar has buttons with 3D conformation figures of ring structures. Errors may be corrected by using the undo feature or the eraser icon on the toolbar. Structures and components not available in ChemWindow can be pasted in from the Windows clipboard. Unlike less sophisticated chemical drawing software, ChemWindow does not limit its user to fixed bond lengths and angles. Users can alter bond length and angle from the default settings with the edit command of the Override Style feature. Structures can also be altered by stretching and twisting them with the shaping tool.

Chemical reaction diagrams are produced easily with toolbar icons that permit the placement of arrows indicating electron flow. Individual components can be dragged and rotated to align with the overall figure. Atoms can be labeled with letters, numbers, Greek symbols, and charges. Any font available through Windows can be imported into ChemWindow diagrams. A useful feature allows tables to be designed to stand alone or be associated with a figure. Thus, comprehensive camera-ready diagrams can be developed for hard copy or storage. Any figure created in the program can be stored in the Windows clipboard and exported to wordprocessor and graphics software for further detailing. One limitation of ChemWindow is that users can only produce wireframe diagrams of molecules with it. The program cannot make ball-and-stick or space-filling diagrams, but one solution is to employ SymApps for other renderings.

Spectral data and chromatogram curves can also be prepared for publication with ChemWindow. Curves can be imported using common file formats (ANDI Mass Spec, Bomem, Bruker, Jasco, Mattson, Shimadzu, and others) found in laboratory instrumentation software and databases. A button on the toolbar makes it possible to import a curve to the window in two steps. New file formats that are not available with ChemWindow can be created by using the filters feature, permitting the program to expand the range of files it can work with considerably. Updated formats are also regularly made available and can be downloaded free from the ChemWindow Web site (www.chemwindow.com/tutorials/filters.html). Once imported, spectra can be modified with the curve editing toolbar. Curves can be reproportioned, rescaled, and flipped. Portions of the curve can be enlarged for extracting more detailed information. Two or more curves can be assembled on the same page, overlaid, and offset for comparative analysis. An annotation tool permits the labeling of peaks with letters or chemical structures.

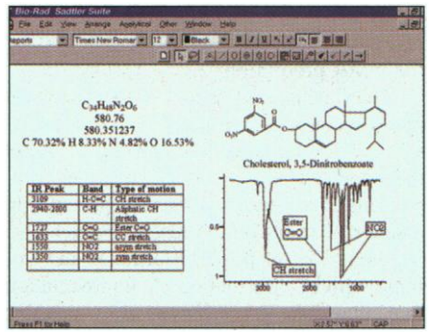

Fig. 1. A report from ChemWindow Spectroscopy complete with structure, IR spectrum with annotated peaks, table with IR Information for each peak, and mass percentage calculations.

ChemWindow's ability to draw laboratory setup diagrams is a novel feature not found in other chemical drawing software. This is very useful for preparing technical reports for submission to safety officers or laboratory managers. A toolbar containing different laboratory equipment icons makes it simple to reconstruct a laboratory bench or design a distillation setup. Images of connectors, condensers, flasks, and thermometers are also available. Large-scale and production figures including reactor designs and piping can be drawn. A tool for freehand drawing is available to modify diagrams.

ChemWindow goes considerably beyond being a contrivance for drawing chemical structures. It also contains useful tools for analyzing drawn and imported chemical structures. ChemWindow can predict ^{13}C NMR spectra and mass spectrometry data for chemical structures created with the program. NMR predictions are presented in a three-part window (Fig. 2). One pane shows a data tree. The other panes show the molecule la-

The author is in the Department of Biology/Environmental Sciences, Kingwood College, 20,000 Kingwood Drive, Kingwood, TX 77339–3801, USA. E-mail: bshmaefs@nhmccd.edu

beled with its associated shift data and a reference molecule used for calculating the NMR prediction.

The Calculate Mass tool of the Analytical menu makes it simple to get mass spectral results. The readout window provides the exact mass and tolerance value. The mass and proportions of component atoms are presented in a series of fields on the readout, which also includes a list of possible formulas and isotopic pattern information. A fragmentation tool allows one to see figures of the possible fragmentation products. The figures can be saved and used to produce graphic displays, or can be exported into text.

Another analytical feature of ChemWindow is the IR correlation feature, which assists in determining if a certain structure matches a known reference spectrum. Data is presented in ChemWindow panes that display the query structure and the reference IR spectra. A functional group pane allows one to match known functional groups to specific peaks. A band pane allows the user to find peaks associated with particular functional groups.

IR SearchMaster

IR SearchMaster is a tool for extracting IR spectra from a database. With the program, users can search an IR library by chemical name, chemical structure, peak properties, or spectrum. Simple, as well as combination, searches can be conducted with little effort. A very useful feature is IR SearchMaster's ability to import Fourier transform–IR data from instrumentation software. IR SearchMaster uses a workspace window divided into three areas. A data view window provides information about the search organized into a tree arrangement. The spectral view window displays the full spectrum as well as the "hit list" window that displays and organizes the matches from a search.

Once a spectrum is obtained, users can adjust baseline bias, remove peaks, smooth to reduce noise, rescale to reset the minimum and maximum, and truncate to reduce the range. Spectra collected and edited in an IR SearchMaster search can be moved into ChemWindow for annotation, labeling, and further modification. The spectra can then be incorporated into publications or electronic laboratory books. IR SearchMaster also links to IR Mentor Pro for calculating peak correlations on the spectra.

Sadtler, which claims to have the world's largest IR spectra database for pure compounds, provides an option to purchase expanded IR library databases. Several are supplied with the main software package. A library access control device, a 25-pin connector attached to the computer's parallel port, is required to use the database. Access is controlled by a license agreement with Bio-Rad. Spectra collected by the online search may be stored to disk as a local library.

IR Mentor Pro

Comparing and analyzing spectral data is the forte of IR Mentor Pro, an online spectral database program that assists in the interpretation of IR spectra. It also serves as a tutorial for instructing neophyte spectroscopists on the basics of IR interpretation. IR Mentor Pro provides a toolbar with buttons to access the software's common functions. The software starts up with a four-part working area, which includes a spectrum window, structure window, a chart window that highlights the bands, and a results window providing identified functional group information.

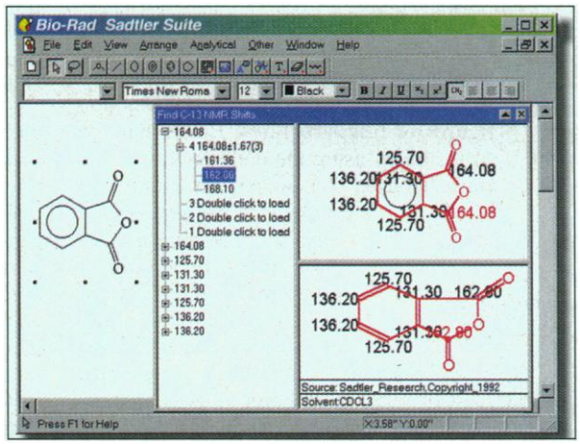

Fig. 2. A ^{13}C Analysis with ChemWindow Spectroscopy's ^{13}C NMR Prediction Tool

The software allows the user to match the peaks of an imported spectrum with a database of probable functional groups. IR Mentor Pro's database includes 600 peaks that correspond to 200 functional groups within the 4000- to 400-cm range.

IR Mentor Pro can be used in several ways to assist with spectral analysis. The correlation function permits a user to find functional groups and bonds that match selected peaks in a spectrum. It can also be used to identify or eliminate components of a chemical mixture by identifying key functional groups on the spectrum. Another application is to use it to quickly assess all the functional groups that can correspond to a particular peak.

SymApps

SymApps is a stand-alone program for creating 3D chemical structure renderings that also is an important companion for ChemWindow, allowing users to convert ChemWindow's wire-frame diagrams into various 3D diagrams. Just like ChemWindow, SymApps opens up to a blank page with a simple-to-use toolbar and large buttons for rotating and magnifying the molecule. SymApps's utility is expanded by accessibility from within Microsoft Word, WordPad, and other programs supporting Object Linking and Embedding (OLE). OLE-compliant applications permit SymApps to operate in the background while they are running.

SymApps is straightforward to use, whether alone or coupled to an OLE application. In SymApps, a chemical structure created with ChemWindow is first entered from the clipboard. (SymApps can also open files in MDL, PDB, XYZ, Mopac, and Gaussian Z-matrix formats.) Wire-frame figures can then be converted to a ball-and-stick or space-filling renderings using the Render menu. Atoms can be color-coded after a rendering is generated. New renderings can be stored as 3D files for later use. A useful visualization feature is a menu that permits a user to hide a selected element or group of elements, allowing one to see structures normally covered up by other components.

Summary

Sadtler Suite is a very versatile software package designed for broad usage. The package excels at producing publication-quality chemical structure figures and does a good job performing spectral analyses. The software is equally at home in research and production laboratories. Though its utility as a versatile chemical graphics package alone would make it a worthwhile investment, the spectroscopy functions have been nicely integrated to make the Sadtler Suite a very welcome comprehensive chemistry product.

System Requirements

Sadtler Suite requires a minimum of a 486 Windows-compatible PC running either Windows 95, 98, or NT. A Pentium with at least 24 MB RAM is highly recommended. This allows the software to run quickly and prevents seizing of the system when carrying out calculations.

The software loads from a CD-ROM and takes up 40 MB of hard drive space. A modem for downloading data or structural files from the Internet is also helpful to make full use of the software. Sadtler Suite was tested on a Compaq Pentium II 350 MHz CPU with 64 MB RAM and a DVD CD-ROM. It used a DOS 7 operating system running Windows 98.