TECHSIGHTING
SOFTWARE

e-Reference Tool

Bibliographic software is a must-have product for anyone preparing scientific manuscripts. Well-designed reference management packages, such as Reference Manager 9, search the Internet for relevant literature, create a database, and reformat the references to fit the style needed for a manuscript. Much of the power of Reference Manager 9 lies in its "cite while you write" capability, enabling users to import references into a document without leaving their word processing program.

Reference Manager 9
ISI ResearchSoft
Berkeley, CA
$356, institutions; $99, students
510-559-8592
www.risinc.com

Reference Manager 9 automatically integrates into word processing software (Microsoft Word for Windows 7, 97, and 2000 and Corel WordPerfect for Windows 7, 8, and 9) as a toolbox item under the Tools menu. This allows the user to access Reference Manager's functions to search for, import, and edit citations within their word processor.

Adding a citation to an active document is simple: First, open a bibliographic database created with Reference Manager by choosing the Open Database menu from the Reference Processor tool bar. A two-part reference window then shows a list of articles in the database in one pane; the other displays detailed information on any item selected.

Next, chose a reference from the database and format it into the publication's desired reference style. Reference styles available in Reference Manager 9 may be viewed at www.refman.com/outputstyles.html. References can be sorted and further customized during this operation. Once edited, you can print your reference list, import it into another database, store it on disk, or insert it into a manuscript.

Creating a new database simply involves opening the Database window and customizing the options for managing references. Articles for the database can be retrieved by searching CD-ROM and online bibliographic sources. The completed database can be stored on the user's hard drive or on an external disk. Reference Manager allows one to call up several databases simultaneously when working on a document.

Reference Manager can import a variety of file formats from over 140 commonly cited scientific journals. Its search engine can access popular CD and online databases such as Datastar, Dialog, Knowledge Index, SilverPlatter, UMI, and Wilson. Version 9 also searches the powerful PubMed and other Internet libraries worldwide, as well as social science and legal periodical databases.

Reference Manager 9 is not solely designed for scientists. It is also useful for journalists, librarians, science writers, and students needing a simple way to look up citations. Manuscript reviewers will also find Reference Manager 9 handy as a tool for checking references and for locating information on the topic being reviewed. College science instructors can use Reference Manager 9 to provide students with hard copy and online reference lists for class use, and graduate students will find it useful in managing references for a dissertation. It offers features not found in other popular bibliographic software packages, such as flexibility in copying reference information between databases and the ability to search 10 databases at once. The program is valuable for collecting references and organizing large bibliographic databases for a variety of needs. It is highly recommended for anyone needing a powerful referencing tool.

—BRIAN R. SHMAEFSKY

Kingwood College, Department of Biology/Biotechnology, 20000 Kingwood Drive, Kingwood, TX 77339, USA. E-mail: brian.shmaefsky@nhmccd.edu

TECHSIGHTING
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Turning Structures Into Gold

Alchemy 2000 (version 2.05) is a comprehensive molecular modeling program with several advanced tools for real-time graphics visualization and computation of small molecules, material polymers, and biopolymers. It can create molecular structures for export into various formats, making it easy to transfer molecular structures between modeling programs. Alchemy 2000 also has five optional application modules: SciQSAR (quantitative structure-activity or structure-property relationships of small molecules), SciProtein [builds and views proteins in three-dimensional (3D) and effectively predicts secondary structure for a wide variety of biological proteins], SciPolymer (for de novo design and prediction of material polymer properties), SciLogP (predicts small molecules' logP values—a measure of hydrophobicity), and ChemPrint Pro (2D chemical drawings).

Alchemy 2000 can download molecules for display directly from the Internet; build, modify, analyze, and convert 2D chemical drawings of molecules into their accurate 3D representations; minimize energy and optimizing geometry; predict molecular dynamics under controlled temperatures; and calculate molecular properties such as dipole moment, van der Waals volume, and surface area.

Alchemy 2000
SciVision200
Burlington, MA
$995 (commercial)
$695 (academic)
SciQSAR $650
SciProtein $595
SciPolymer $995
SciLogP $495
ChemPrint Pro $150
800-861-6274
www.scivision.com

Quantitative Structure Activity Relationship (QSAR) is an important computational analysis tool for medicinal chemists who design small molecules. The SciQSAR module of Alchemy 2000 designs and predicts the activities and properties of new compounds. It uses several expandable descriptors (e.g., logP, dipole moment, and volume) and can perform automated analysis of hundreds of compounds.

SciProtein provides easy tools for building protein and peptide primary and secondary structures that can be displayed with Alchemy 2000. This module allows sequence similarity searching and motif identification from 3D structures in a database. Hydropathy, antigenicity, and mutability are generated by the module and are useful tools for researchers to investigate protein structure and function.

The SciPolymer module can be used to design polymers based on monomeric units and to predict their properties (e.g., cohesive, electrical, optical, and thermal). It has an extensive polymer-property database of 659 polymers, which can be used for the development of the next generation of polymers. Of all the optional modules for Alchemy 2000, SciPolymer has the most thoroughly designed interactive database.

SciLogP has five built-in regression equations for the prediction of logP values (octanol-water partition coefficients) that can be used with the internal regression analyzer.

Overall, Alchemy 2000 is useful for building and visualization of small and large molecules (e.g., proteins and polymers) and could be used effectively to teach chemistry in classrooms. Serious drawbacks include the fixed setting of force fields and the absence of graphic display of

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molecular orbitals, but the integration of the optional application modules (SciQSAR, SciProtein, SciPolymer, and SciLogP) is a strength. Alchemy 2000 and the application modules run under Windows 95, 98, or NT.

—RAMA K. KONDRU AND ASHVANI K. SINGH

R. K. Kondru is in the Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260, USA. A. K. Singh is in the Department of Cell Biology and Physiology, University of Pittsburgh, Pittsburgh, PA 15260, USA. E-mail: asingh+@pitt.edu

TECHSIGHTING
SOFTWARE

Origin Update

Origin 6.0 is the most recent version of the popular data analysis and graphics software developed by Microcal. The major enhancements to this version of Origin are the Project Explorer, drag-and-drop plotting, data masking, expanded graphics export, and customizable toolbars. The Project Explorer is a Windows Explorer-like interface within the program. It allows one to create folders within a project to categorize data, graphs, or results, thus not only reducing project loading time, but also allowing the user to find and open files very quickly. The drag-and-drop plotting feature can quickly plot data identified by highlighting the desired columns and dragging to the plot window. Data masking with the Mask toolbar allows one to temporarily exclude outliers or specified data ranges during data analysis and to color code or hide the masked data.

Origin 6.0
Microcal Software, Inc.
Northhampton, MA
Origin 6.0, $595;
Origin 6.0 Professional, $895
413-586-2013
www.microcal.com

The versatile import and export formats supported by Origin 6.0 make it compatible with numerous other data acquisition, analysis, and presentation or publication applications. A pClamp module, used to read Axon binary files, is built into Origin 6.0. Additional formats supported by Origin 6.0 include Excel; Lotus; dBase; DIF; WAV; Mathematica vectors and matrices; LabTech; KaleidaGraph; Encapsulated Postscript (EPS); Adobe Illustrator (AI); Enhanced Metafile (EMF); Computer Graphics Metafile (CGM); Bitmap (BMP); Tag Image File (TIF); and Adobe Photoshop (PSD) formats.

Origin 6.0 has numerous built-in graphical plot types. These include simple line and scatter plots, vector plots, polar and ternary plots, three dimensional (3D) color-mapped surface and contour plots, and 3D pie charts. Line thickness, symbols, and other graphical display properties can easily be modified from the new Plot Details dialog box. The ability to layer plots and to link those layers and axes continues to be one of the most useful features of Origin. Multiple layers and graph axes can be linked so that changes in scaling for one layer are automatically applied to the other linked layers. The template functions in Origin enable one to create and save frequently used data analysis and graph formats. This, along with the Origin scripting language, LabTalk, can facilitate analysis of large data sets.

The built-in Origin 6.0 data analysis tools are numerous and include descriptive statistics, *t* test, analysis of variance (ANOVA), linear regression, baseline and peak analysis, Fast Fourier Transform (FFT), smoothing, filtering, and calculus operations. Nearly 200 built-in fitting functions can be executed by the Origin nonlinear least squares fitting algorithm. The graphical interface for nonlinear fitting displays equations and sample curves for selected functions. In addition, user-defined functions can be written for nonlinear least squares fitting within Origin. Unfortunately, in this version, LabTalk scripting can no longer be used for data acquisition.

The product technical support is extensive and includes free telephone support, software manuals, online help, and a discussion forum for posting technical and trouble-shooting issues. In addition, patches that fix program "bugs" are available at the Microcal website, as are program add-ons and LabTalk scripts written by other Origin users. The Origin 6.0 manuals and tutorials that come with the software are very well written and helpful.

—KATHY E. MITCHELL

Department of Anatomy and Physiology, 1600 Denison Avenue, Kansas State University, Manhattan, KS 66506, USA. E-mail: mitchell@vet.ksu.edu

TECHSIGHTING
SOFTWARE

Eye on the Sky

Distant Suns software brings the heavens to the screen of a personal computer. Designed primarily as a learning tool for interested amateur astronomers and college-level students, the program superbly delivers a great number of features in a product that is easy to use. Distant Suns avoids the explicit use of mathematics while providing good explanations of many astronomical phenomena.

At startup, the screen displays a view of the night sky centered on the pole star for the current date, time, and location. Three buttons provide easy access to useful program functions: the planetarium (the main feature of the program, which shows astronomical displays), the grab bag (a collection of relevant astronomical facts), and the calendar feature (which allows the viewer to move forward or backward by months to locate astronomical events). Other buttons will set the sky to appear as it would at sunrise or sunset of a given day or to center the view looking north or south. The sky can be observed from many perspectives, centered on the sun or moon, or on an arbitrary point in space. Names of planets and Messier objects can be toggled on or off, as can constellation lines. User-adjustable clock functions control animations of planetary motions that can be sped up, stopped, or reversed. Another button illustrates what the developers feel are the "best" deep sky objects.

Distant Suns 5.1
Monkey Byte Development, LLC
San Luis Obispo, CA
$34.95
800-522-3774
www.monkeybyte.com

The program can display special effects such as eclipses, planetary motions, asteroid approaches, and other solar system events. Orbits can be plotted for objects, the next meteor shower information is easily identified, and a user-positionable tool palette allows instant access to planetary views and data. For the latest discoveries, Distant Suns maintains an up-to-date website. Both NASA's Skymap and Hubble Guide Star Catalog were used in the program's database, so over 21,000 stars are available. All 110 Messier objects are included as well as 1500 of the objects from the New General Catalog (NGC). There is more than enough power to keep the average undergraduate astronomy class profitably occupied and the amateur astronomer delighted.

The program lacks a preprinted manual, but a complete reference guide may be printed from the CD-ROM. It contains instructions for using the program; explanations of astronomical terms and concepts; a guide to the solar system, stars, and deep sky objects (galaxies, clusters, and nebulae); the Messier Catalog and abbreviated NGC catalog; brief tables of planetary data and meteor showers; and a list of references. It even contains a section on buying a telescope. Many photographs and diagrams are included, some in color. Although brief, the explanations in the reference guide will go far to supplement the usual textbooks. Overall, Distant Suns is a very worthwhile learning guide at a great price.

—JOHN A. WASS

Abbott Laboratories, Abbot Park, IL 60045, USA. E-mail: John.Wass@add.ssw.abbott.com