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

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TECHSIGHTING
SOFTWARE

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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