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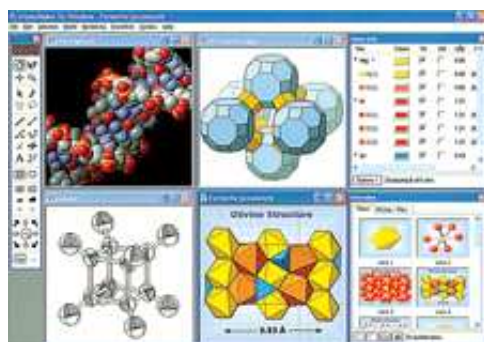
p. 38

Digital Briefs

New Software and Websites for the Chemical Enterprise

Software

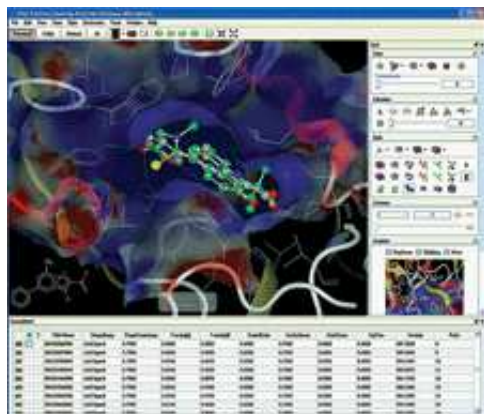
The following are some of the products that were on display at the exposition during last month's American Chemical Society national meeting in Boston.



1

(1) CrystalMaker is a program for fully interactive visualization and analysis of crystal and molecular structures. The software features real-time manipulation of structures; photo-realistic graphics and 3-D stereo; digital video, animation, and QuickTime Virtual Reality output; and a crystal structure library. CrystalMaker lets the user work with multiple structures and views; rotate structures interactively with the mouse or keyboard; measure bond distances and angles using on-screen tools; display lattice planes and generate crystal faces and surfaces; hide or repair molecular fragments and isolate individual molecules; and combine multiple structures in "molecule mode." Available for Mac OS X and for Windows XP. **CrystalMaker Software**, www.crystallmaker.co.uk

KnowItAll U is a spectroscopy resource for academic research and teaching that includes more than 1.3 million NMR, IR, UV-Vis, Raman, and mass spectra. These data cover pure compounds as well as a broad range of commercial products used in pharmaceutical, forensic, polymer, and environmental chemistry. Database records are searchable by parameters such as full spectrum, peak, structure, substructure, name, and molecular weight. A site license also includes KnowItAll AnyWare, a platform-independent Web browser interface to the KnowItAll U database collection; an informatics system that includes structure drawing, reporting, processing, data mining, chemometrics, and NMR spectra predictions; and SpectraBase, a community reference spectral database. **Bio Rad**, www.knowitallu.com



2

(2) Vida is a graphical user interface that visualizes, analyzes, and manages large sets of molecular information. It supports all standard visualization paradigms, including 2-D depiction, hardware and software stereo, and surface selection and manipulation. Vida features a chemically oriented, fully functional spreadsheet; automatic browsing facilities; support for most industry standard file formats; real-time contours; 3-D display and graphs; and electrostatic grids and electron density maps. With the Vivant tool, users can import files into Microsoft PowerPoint and animate the file via 3-D interaction. The software is supported on Windows, Linux, Mac OS X, and IRIX systems. **OpenEye Scientific Software**, www.eyesopen.com

CheVi v.6.1 is a chemical visualizing package designed to give insight into how ligands and receptors interact. The user can visualize receptor binding site characteristics, in which the color-coded receptor surface dramatically displays the characteristics of the binding site, and ligand properties, in which the surface of the ligand can also be visualized to show the chemical characteristics of the ligand. The software also visualizes key receptor-ligand interactions, whereby showing strong interactions between ligand and receptor with color-coded dashed lines can give valuable information on how and why a ligand docks in a particular position. CheVi has a Web-based user interface with 3-D capabilities and has an export capability for high-resolution, publication-quality images. The software is currently available on Linux and will soon be available on most other platforms. **Simulated Biomolecular Systems**, www.simbiosys.ca



3

Sylvia provides a method to rapidly evaluate the synthetic accessibility of chemical compounds and to prioritize thousands of structures according to their synthetic complexity. In its calculation process, Sylvia integrates various structural and chemical features of the target molecule that are contemplated when chemists manually evaluate the synthetic accessibility of a set of compounds. The software ranks chemical compounds on a scale that reflects whether a structure can be synthesized by a straightforward synthesis route or whether it is a complex, challenging synthesis target. The software can effectively be incorporated into virtual screening tools or de novo design systems to rank large amounts of structures according to their synthetic complexity. Sylvia is available for Windows and Linux systems. **Molecular Networks**, www.molecular-networks.com

Palmtop

(3) Vernier LabQuest is a data-collection palmtop device with a rechargeable battery and full-color, touch-screen capability. It works with existing Vernier sensors; is splash proof with a rugged design; has built-in sound and temperature sensors, as well as graphing and analysis software; and is equipped with applications such as a stopwatch, color-coded periodic table, and scientific calculator. The device performs linear and curve fits and features autoscaling, integral functions, and statistical analysis. LabQuest can be used as a computer interface, a stand-alone device, or in the field. **Vernier**, www.vernier.com

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