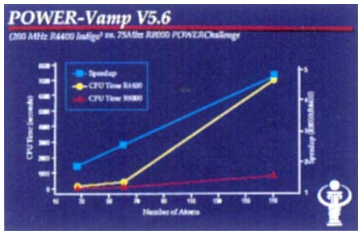
Setting the sights on software

Marketplace highlights a selection of new and useful products to the broad sweep of scientists interested in structural biology. We also welcome suggestions for future features.

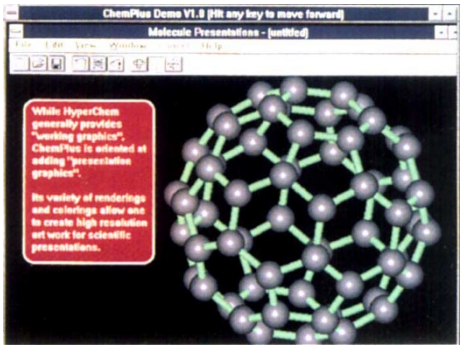
The relentless advance in new and ever more powerful processors and sophisticated computer platforms demands an equally rapid development of software products—such that the utility of the program(s) and the capability of the processor(s)/peripherals are maximized.

To this end **Oxford Molecular** have now optimized its computational chemistry software for Silicon Graphics systems based on the MIPS® R8000™ processor. The latest version of the AMBER molecular mechanics simulations software, POWER AMBER, takes advantage of the floating point speed of the R8000 CPU and Silicon Graphics shared memory capabilities (indeed Silicon Graphics has further improved the software to maximize its performance on multiple processor machines). These features, it is said, allow calculations to be routinely performed on a departmental server that were previously only possible on supercomputers (see *http://www.amber.ucsf.edu/amber/bench.txt*). POWER Vamp, a semi-empirical quantum mechanics (QM) program for studying the characteristics of large molecules, as well as notching up a fourfold improvement in performance with the R8000 provides—among other things—a mixed QM/molecular mechanics model that can be used to study drug–protein interactions, an experiment that until now has not been possible to perform using existing QM techniques, the manufacturers say.



Fast and furious—the latest version of Power Vamp and Power Amber.

The new ChemProtein module for Chem-X, developed by **Chemical Design Ltd.**, allows users to build 3D models of their chosen target protein by a process of automated homology modelling. The modular architecture of Chem-X software means that results generated in ChemProtein can be further analysed by an array of database and modelling tools, including energy minimization, dynamics, and docking protocols, the manufacturers say. Chem-X is also available to users of the Microsoft Windows® 95 operating system. For those working with slightly smaller molecules, such as peptides and nucleic acids and even highly coordinated metal complexes, Hyperchem, the molecular modelling software from **Autoscribe Ltd**, is said to provide an easy-to-use, comprehensive, integrated set of tools for studying and predicting molecular properties. Molecular structures can be imported from several file formats, such as the PDB, MDL MOL and Sketch and Tripos MOL2 files.



Hyperchem–for modelling smaller molecules.

As well as providing tools in their own right, computers and their associated software provides essential support for many technical applications. **Beckman Instruments Inc.** now introduce their chromatographic workstation software, Gold™ *Nouveau*, for control of, and data acquisition from its System Gold *Nouveau* HPLC instruments. Features offered by the software—which runs under the Microsoft Windows® operating system—include: direct control; method editing; multi-sample automation; post-run chromatogram manipulation and display; and diode array detector graphics. Gold™ *Nouveau* also offers options for multiple data transfer, customized report formatting and password protection.

Computer controlled HPLC from Beckman Instruments, Inc.

Keeping track of the ever expanding scientific literature, even in the most specialized of research fields, requires a highly organized, computerised, filing system that provides easy and convenient access, especially when putting together reports, papers grants and that science book you always promised you were going to write. The latest software upgrades of EndNote (EndNote Plus 2.0) and Endlink (2.0) from **Niles and Associates**, as well as supporting Windows® 3.1, 95 and NT, have (among a series of upgraded features) large collections of pre-defined templates; Endnote Plus 2.0 includes more than 200 bibliographic formats for different journals (including in their number *Nature Structural Biology*) and Endlink 2.0 has more than 100 'filters' for importing references from popular on-line services and CD-ROMs.

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