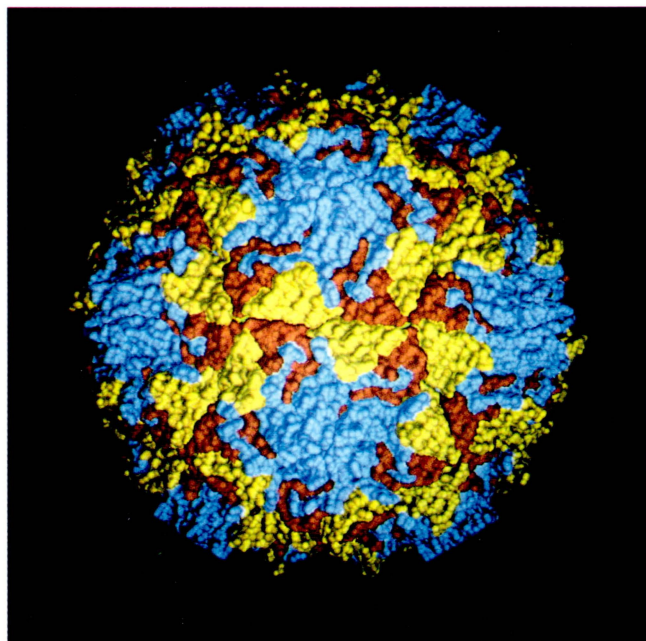


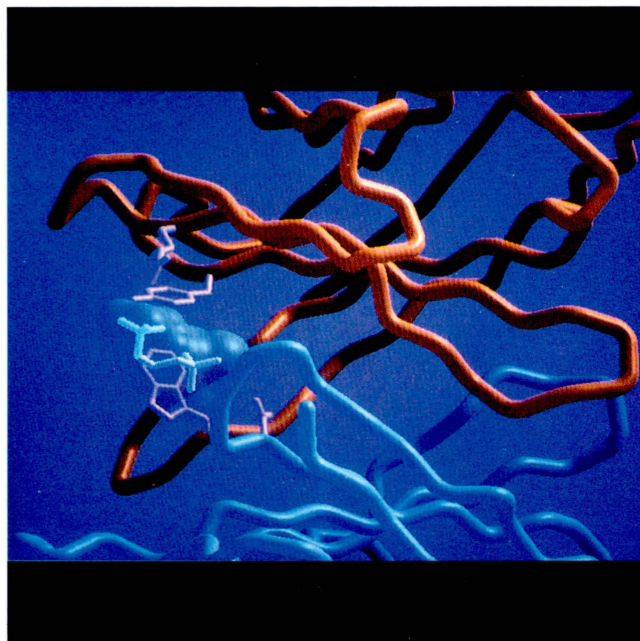


CONVEX

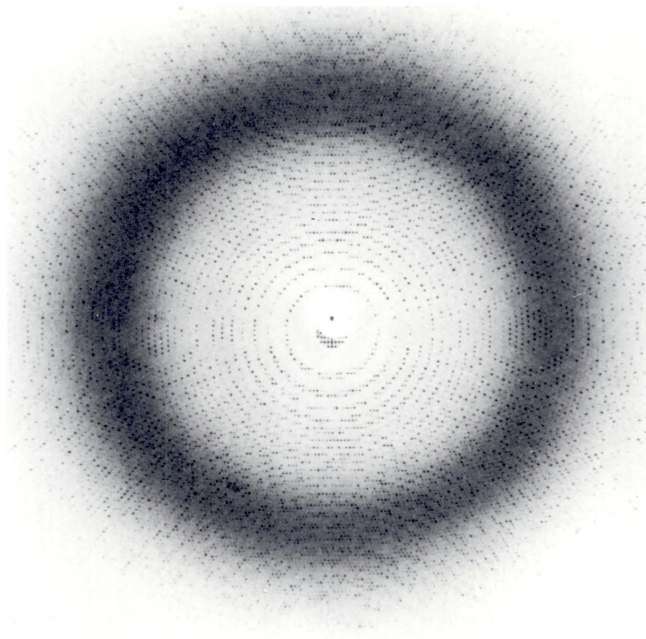
# COMPUTATIONAL MOLECULAR BIOLOGY: An Applications Profile from Convex Computer Corporation



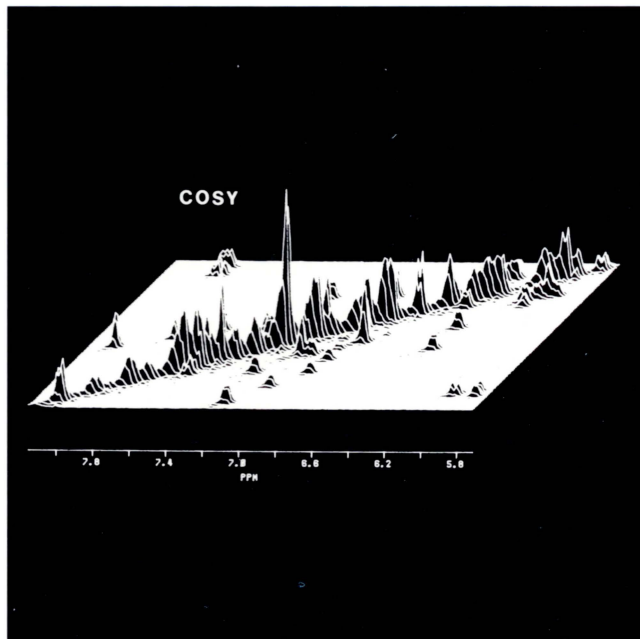
Computer graphics representation of the structure of the poliovirus, which was solved by x-ray crystallographic method by J. Hogle, M. Chow, D. Filman. Figure prepared by A.J. Olson.



This image represents the binding interaction between an antibody combining site and a hapten antigenic molecule. Model by A.J. Olson; structure from D. Davies, National Institutes of Health.



X-ray diffraction photograph from a crystal of the Sabin strain of type 3 poliovirus. Photograph by J. Hogle.



A small region of a two-dimensional nuclear magnetic resonance spectrum of a protein.

The Research Institute of Scripps Clinic is one of the country's leading biomedical research institutions. The Institute undertakes pathbreaking research concerning the structure of molecules, their interactions, their relationship to the immune

system, and their relationship to disease and its cure. Through an extensive and widely respected post-doctoral fellowship program, the Institute is also a premier educator of new generations of scientists.

## THE PROBLEM

Sophisticated analytic techniques and high-performance computer systems have advanced the frontiers of biomedical research, making possible at Scripps such significant discoveries as the solution of the three-dimensional structure of the poliovirus.

In recent research on macromolecular interactions, Institute scientists used computer graphics to analyze crystallographically determined protein structures. Models of molecular shape, electrostatic forces, solvent structure, and patterns of mobility organized the data to allow recognition of previously unnoticed relationships and patterns. Based on the insights derived from this modeling, researchers are seeking to integrate the properties into a model of protein structural and functional interactions, and to devise specific and useful experiments.

As this example suggests, the Institute's research evolves and expands as changing technologies and techniques open new avenues of investigation. The principal factor determining the Institute's computing needs nevertheless remains constant: in order to sustain its leadership in biomedical research, Scripps must have computing resources sufficient to develop and run software that requires large amounts of memory, high computational speed, and a high I/O bandwidth speed.

In 1985, the Institute's Department of Molecular Biology, which was using a standard minicomputer to determine and model molecular structures for basic molecular biological research, found that its performance needs were rapidly outgrowing existing resources. The runtime on minis far exceeded acceptable turn-around and the size of the problems required more memory than the current hardware system provided.

One option was to purchase a newer, faster minicomputer. It seemed evident, however, that the Department's needs would quickly outstrip the capabilities of that system as well, resulting in a series of upgrades to the ever-higher levels of minicomputer performance. To avoid this cycle of installation and replacement, the Institute began a search for a system that could handle its long-term computing needs.

## THE SOLUTION

The Research Institute of Scripps Clinic found its solution in the Convex C1 supercomputer, a 64-bit, integrated scalar and vector processor.

A critical element in the Institute's decision was the C1's Cray®-like architecture. Because of the architectural similarities, algorithms used to design software on the C1 are the same as those used to develop software on the Cray. The Institute, which

has access to the Cray located at the Supercomputer Center at the University of California at San Diego, develops much of its software in-house on the Convex and runs it on the Cray.

In addition, the Convex C1's large physical memory size (128 MBytes), its high I/O bandwidth speed (80 MBytes a second), and its speed of computation addressed the Institute's concerns with current equipment and future upgrades.

The C1 delivers performance up to 20 times faster than the Institute's minicomputers. The scientists at Scripps found they could do multiple program runs per day on a system that offers supercomputer performance, UNIX®, VAX™/VMS™ FORTRAN compatibility, and ease of conversion of the existing software base.

The C1 is used in the experimental and the theoretical analysis conducted by Scripps. It aids the determination of a structure using x-ray crystallography and is also involved in the three-dimensional modeling of molecular structures.

## THE ORGANIZATIONS

The Research Institute of Scripps Clinic, part of Scripps Clinic and Research Foundation, is located in La Jolla, California. One of the country's leading biomedical research institutions, the Institute conducts research on the structure of molecules, their interactions, their relationship to the immune system, and their relationship to disease and its cure. The Institute has three major divisions: the Department of Basic and Clinical Research, the Department of Immunology, and the Department of Molecular Biology.

Convex Computer Corporation is headquartered in Richardson, Texas, and was founded in September 1982 to design, manufacture, market, and service affordable supercomputers for a wide range of technical users. The company's

first product, the Convex C1, began shipment in March 1985. Convex has sales and support facilities worldwide. The C1, which features a Cray-like architecture, combines the memory and vector processing capabilities previously found only on supercomputers with the software advantages and price of minicomputers.

**“Advances in biotechnology are diminishing the interval between scientific discovery and commercial application.**

**In this environment, the leaders in biomedical research are those who can focus first-rate scientific talent on the major issues in the field — and who also take full advantage of powerful new tools such as the Convex C1 supercomputer.**

**Convex, like Scripps, is at the vanguard of its technology. The C1 system exceeds anything in its class in performance, memory capacity, and in software support.**

**With the C1 in place, we can spend less time waiting for the completion of software simulation runs and more time in productive research.”**

**Richard Lerner, M.D.,  
Director, Research Institute  
of Scripps Clinic**