IBM

Structural Bioinformatics supports drug discovery with IBM and Linux.

Overview

■ **Challenge**

   Offer customers highly available, reliable computing services with increased processing speed and capacity at lower cost

■ **Solution**

   Drug discovery data management solution designed to identify and store three-dimensional protein structures

■ **Why IBM?**

   SBI read positive reports about the versatility, scalability and performance of IBM DB2® Universal Database™ and valued IBM's support and commitment

■ **Key Business Benefits**

   Cost per calculation reduced from $28 to $1; 75% increase in computing capacity; superior speed, performance and scalability of DB2 compared to other databases; initial development completed 6 months ahead of schedule; faster, easier development of new applications

■ **Business Partner**

   Direct Solutions Support
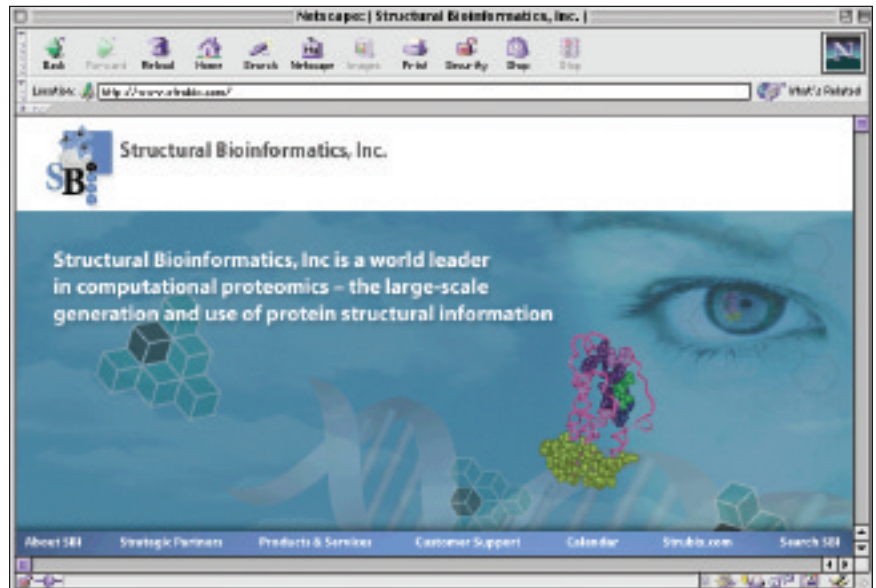
More than half of Structural Bioinformatics' 100 employees hold Ph. D. degrees in disciplines such as physics, biophysics, mathematics and biochemistry.

Computational proteonomics isn't exactly a household phrase, but it is a lifesaver nonetheless. One company that understands this is San Diego, California-based Structural Bioinformatics, Inc. (SBI), a world leader in computational proteonomics and the use of protein structure information to develop drugs that treat such illnesses as cancer and cardiovascular disease. Computational proteonomics involves performing computations on protein gene sequences to identify their three-dimensional structure.

"Modeling a protein requires a series of massive calculations, which previously could take as long as 14 hours each. It was an expensive process that kept our cost structure high."

– Ed Maggio, CEO, Structural Bioinformatics, Inc.

e-business

Key Components

Software

- IBM WebSphere® Application Server, Advanced Edition, Version 3.5
- IBM DB2 Universal Database Enterprise Edition for Linux®, Version 7.1
- IBM DB2 Universal Database for Microsoft® Windows NT®
- IBM DB2 OLAP Server™
- IBM DB2 XML Extender
- IBM DiscoveryLink™

Servers

- IBM @server xSeries™ 230

"We see a marked improvement in performance with DB2 compared to Oracle — our computing capacity has increased 75 percent."

–Dr. Kal Ramnarayan, Chief Scientific Officer, Structural Bioinformatics

The reason for SBI's success is crystal clear: All drugs target specific proteins, and pharmaceutical companies must understand three-dimensional protein structures in order to formulate their remedies.

Seeking to offer its customers faster, better services at lower costs, SBI wanted to migrate its protein-modeling system from an infrastructure based on Oracle and Sun to a solution that would provide more processing speed and capacity with higher availability and reliability. After hearing positive reports about IBM DB2 Universal Database and Linux running on Intel processor-based servers, SBI decided that DB2 for Linux and Linux clusters of IBM @server xSeries servers would be its next solution, along with IBM WebSphere Application Server for delivering transactions over the Web.

This choice paid off immediately. As SBI CEO Ed Maggio explains, "The combination of Linux, DB2 and xSeries servers increased our cost-efficiency. Modeling a protein requires a series of massive calculations, which previously could take as long as 14 hours each. It was an expensive process that kept our cost structure high." Adds Ralph Barry, chief financial officer for Structural Bioinformatics, "For one series of calculations, the Linux operating system combined with IBM hardware and DB2 helped reduce our benchmark costs from about $28 per calculation to below $1. Now we can afford to raise the bar to even greater levels of structural refinement."

Other benefits have been equally as dramatic. "We see a marked improvement in performance with DB2 compared to Oracle — our computing capacity has increased 75 percent," says Dr. Kal Ramnarayan, chief scientific officer for Structural Bioinformatics. "The IBM DB2 platform has the horsepower to make rapid comparisons of tens of thousands of protein structures."

Hastening the drug discovery process

Typically, a drug company approaches SBI to calculate the protein structure of a particular gene sequence. A second line of business for SBI is compiling and maintaining a database of protein structures, which pharmaceutical and biotechnology companies can access and study online. Companies that want to compare structural characteristics and conduct other analyses access the database over the Internet, using secure passwords and user IDs. WebSphere Application Server sends data back and forth between the customers' systems and DB2 Universal Database. A plug-in toolkit viewer allows users to see the proteins in three dimensions.

Says Ramnarayan, "Our users are extremely sophisticated and want continuous availability. The redundancy and reliability of our IBM solution allow us to provide high performance at a lower cost."

Harnessing computing power with DB2 and Linux

SBI's new system includes a cluster of 64 dual-processor xSeries servers running Red Hat Linux 7.1. The servers are clustered at the application level and communicate with each other over TCP/IP connections. DB2 Universal Database Enterprise Edition for Linux, Version 7.1 resides on two other dual-processor servers, and WebSphere Application Server, Advanced Edition, Version 3.5 runs on still another. High-powered IBM demonstration laptops, used by sales staff to demonstrate SBI technology, run DB2 for Windows NT. SBI also uses IBM DB2 OLAP Server for multidimensional analysis and IBM DB2 XML Extender to gather information about proteins, which appears in various formats on the Web. IBM DiscoveryLink allows SBI to conduct more efficient analyses by searching its numerous databases with a single, optimized query.

In selecting DB2, SBI didn't formally evaluate other alternatives because it had done extensive research on IBM's product direction. "We read about the versatility, scalability and performance of DB2 and followed IBM as its commitment to e-commerce and other client/server applications unfolded," recalls Ramnarayan.

"For one series of calculations, the Linux operating system combined with IBM hardware and DB2 helped reduce our benchmark costs from about $28 per calculation to below $1. Now we can afford to raise the bar to even greater levels of structural refinement."

– Ralph Barry, CFO, Structural Bioinformatics
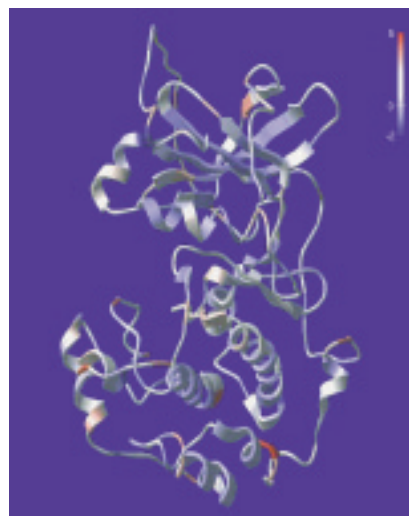
Powered by IBM DB2 Universal Database Enterprise Edition, SBI's ProMax database provides pharmaceutical researchers with structural information on proteins that can be used to develop new drugs.

Porting SBI's applications to DB2 on Linux went without a hitch, enabling SBI to complete its migration six months ahead of schedule. "We thought we would have to use a contractor to assist with the DB2 implementation, but our staff came up to speed very quickly," explains Barry. "With its support for stored procedures, DB2 is easy to work with."

IBM Business Partner Direct Solutions Support provided hardware services, racked and stacked the servers and cabled them together. "We wanted everything, including the Linux operating system, installed and tested offsite so that it would be plug and play when it arrived here," notes Ramnarayan. "And a turnkey solution is exactly what we got."

The scalability that DB2 provides will be important also, given that the SBI database already stores data on more than 100,000 protein structures—and that a file for a single protein can be as large as 30MB. Adds Barry, "IBM's server platform is as scalable as its software. Even if we need to add another 120 processors as our business grows and expands, it's a very simple, efficient and cost-effective process."

Primed for future applications

While no one can say where the fast-changing drug discovery business will lead, SBI is confident that it will have the computing power it needs to meet whatever challenges lie ahead. The user-friendly development environment provided by DB2 will also benefit the company as it creates new applications.

Says Ramnarayan, "Linux makes an ideal platform for integrating DB2, WebSphere and other IBM middleware products because it is compatible with Java™ and other open-standards-based technology. IBM's platforms—both hardware and software such as DB2 and WebSphere—offer reliable, high-performance, scalable product lines with a solid roadmap into the future. We can't see any reason not to go the distance with IBM."

IBM.®