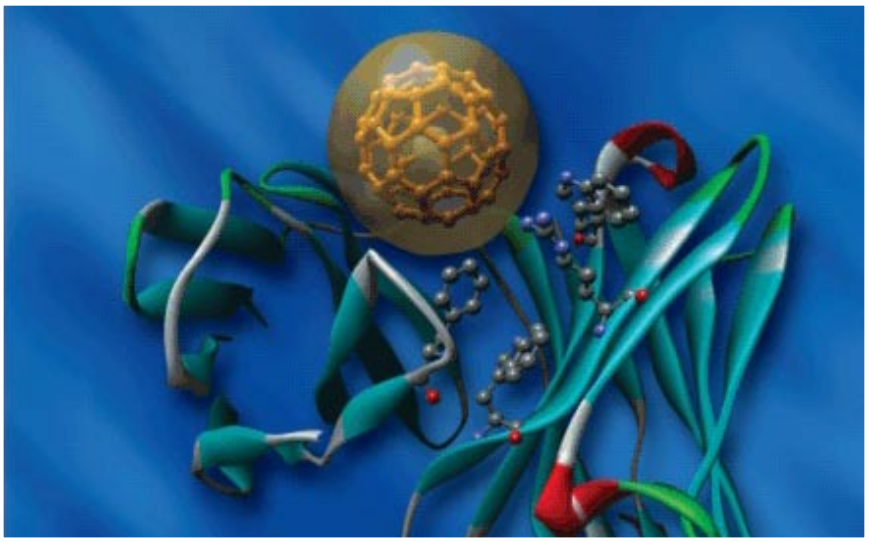
Accelrys and IBM help customers accelerate drug discovery and development



Discovery Studio® from Accelrys was used to analyze the interactions of protein residues (ball and stick representation) involved in the binding of a bucky ball (encased in a binding site sphere).

The success of life sciences companies depends on their ability to characterize more therapeutic targets, develop more drug candidates, reduce attrition in clinical trials and, ultimately, take successful drugs to market faster—all while simultaneously controlling costs. To achieve all this, they must make difficult, interdependent decisions based on capturing, creating and analyzing vast amounts of critical data. This sheer volume of data represents both a major opportunity and a tremendous management challenge; facilities in multiple, global locations further complicate workflow and communication. And mergers, acquisitions, the retirement of experienced staff, increased labor mobility and the dynamic nature of demand make change a constant.

In this complex environment, most companies have recognized the importance of using informatics systems to manage, share and mine data, as well as computational tools to generate and analyze it. But to significantly impact the success of research organizations, these systems and tools must be easily accessible and scalable—from standard desktop and

IBM Business Partner: Accelrys

Accelrys, a leading provider of software and service solutions for life and materials science research organizations, delivers software for the modeling, simulation and management of scientific data used for drug discovery and drug development, as well as product design. Among the company's offerings are solutions tailored to the needs of biologists and chemists working in today's demanding research organizations. Scientific innovation, product development and collaborative projects at Accelrys are driven by teams based out of the company's centers of excellence in San Diego, CA; Cambridge, UK and Bangalore, India. Accelrys has over 470 employees, including more than 200 Ph.D. scientists, supported by an expert software development team.

laptop computers to high-performance computing (HPC) platforms. They must also be tailored to the R&D process and interact with each other and with laboratory information management systems (LIMS), to support the working practices of individual organizations. Equally important is that they are adaptable, compliant with industry and corporate standards and backed by an open IT infrastructure so that organizations can protect their IT and research investments.

Sophisticated solutions

Accelrys offers technology and services in:

- *Simulation and modeling for life sciences research*
- *Bioinformatics and gene sequence analysis*
- *Informatics for HTS and decision support*
- *Chemical information management and data content*
- *Data pipelining and workflow solutions*

Accelrys' premier protein modeling, simulation and structure-based design (SBD) environment—Discovery Studio—provides researchers with a comprehensive suite of solutions for drug discovery and optimization. Key features include:

- *A consistent, easy-to-use interface that can be streamlined based on user need*
- *Open architecture for creating customized business solutions that integrate third-party products or in-house solutions into the Discovery Studio environment*
- *Flexibility for sharing protocols and data from diverse applications to facilitate team communication*
- *Modular design of architecture to maximize the use of IT investments*

Other life science modeling and simulation solutions offered by Accelrys include:

- *Catalyst®, an integrated pharmacophore and 3D database management environment for fast and efficient lead discovery, hopping and optimization*
- *Cerius²®, a collection of rational drug design and SBD tools for accelerating lead design and generation*
- *Insight II®, a collection of best-of-breed algorithms for molecular dynamics, homology modeling, de novo design and electrostatics*
- *QUANTA®, automated and integrated X-ray tools for model building and de novo tracing that help researchers focus their time on structure analysis*

All of these solutions from Accelrys are supported on Linux®-based servers, to support a low-cost and high-performance environment.

Accelrys also offers SciTegic® data pipelining technology. This technology simplifies high-throughput data analysis and mining by letting users automate multi-step, real-time analyses. Users can quickly and easily integrate complex analysis components that run on Linux-based servers, such as chem-informatics components for searching and analyzing chemical structures and

"Our mutual customers' need to deliver innovative pharmaceuticals and products to a demanding market is the driving factor behind this partnership. By combining Accelrys' scientific and software expertise with IBM's middleware and hardware, we can provide a powerful IT infrastructure that organizations can leverage throughout the discovery and development process."

– Mr. Mark Emkjer, President and CEO, Accelrys

data, bioinformatics components for analyzing and annotating gene and protein sequence data and ADME/Tox components for screening potential drug candidates.

Leveraging IBM systems

Accelrys' broad portfolio of application software takes full advantage of the IBM portfolio of high-performance computing platforms, including IBM IntelliStation® Pro workstations, IBM BladeCenter® and IBM System x™ rack-optimized servers. These platforms feature advanced AMD® or Intel® microprocessors running Linux or Microsoft® Windows®.

Selected BladeCenter or System x servers are also available as IBM Cluster 1350 building blocks. The Cluster 1350, a leading-edge Linux Cluster solution, combines the power of AMD Opteron, Intel Xeon, POWER5™ or PowerPC™ servers and blades with IBM Cluster Systems Management (CSM) for Linux software, IBM storage products and leading third-party networking components to create integrated, flexible, scalable platforms for high-performance computing. Cluster 1350 hardware is delivered configured, tested and ready for software installation. Optional Linux cluster installation and support services are available to help clients build complete, robust cluster solutions.

When used together, Accelrys software and IBM systems deliver reliable results, extensive configuration and feature flexibility, leadership performance and significantly lower total cost of ownership.

Accelrys applications support R&D processes ranging from early isolation of target genes and proteins associated with particular diseases, to synthesizing chemical compounds that work on these targets, to preclinical testing and drug delivery. Accelrys technology is designed and licensed specifically to facilitate the life sciences industry transition from an isolated workstation environment to a collaborative enterprise-computing model. Accelrys also clearly recognizes the need to maintain data integrity, full application access and dynamic scalability in its solutions.

IBM hardware and middleware provide a robust foundation for life sciences research and development solutions. IBM supports the industry's broadest range of hardware, operating systems and middleware, allowing concurrent running of virtually any combination of Linux, UNIX®, Microsoft Windows, DB2®, Lotus®, Tivoli® and WebSphere® applications. This protects the investment in hardware and applications and helps life sciences organizations integrate new systems and critical data wherever they reside in the information technology environment. IBM systems provide reliability and security and are designed to diagnose and repair themselves, as well as configure and manage the multitude of devices used in life sciences.

"This alliance represents one of the most significant and influential relationships for IBM in life sciences. IBM and Accelrys share the common goal of developing innovative technology solutions that benefit the life sciences community and accelerate drug discovery and development. Our relationship leverages IBM's broad range of high-performance computing technologies and Accelrys' broad software expertise to drive new levels of productivity in pharmaceutical R&D."

– Dr. Caroline Kovac, General Manager, IBM Life Sciences

Advancing R&D

The main goal of the global alliance between Accelrys and IBM is to enhance drug research and development operations by creating a collaborative information technology environment that allows new drugs to be developed faster, more efficiently and at lower cost. Accelrys and IBM scientists and technicians are collaborating to take advantage of ways that their respective technologies and services can be coordinated and enhanced to support the efforts of research organizations worldwide.

About IBM

The goal of IBM Healthcare and Life Sciences is to rapidly bring IT solutions to customers and IBM Business Partners in the fields of pharmaceutical research, biotechnology, genomics, health and other life science industries. IBM is a proven leader in data integration, supercomputing, high-performance storage, e-business and information technology services.

Long-term projects at IBM Research Centers and the IBM Deep Computing Institute foster collaboration with life science companies—bringing domain expertise and innovative technologies to the development of life science solutions. IBM actively collaborates with companies like Accelrys, whose domain knowledge, products and resources can help build valuable solutions for our mutual customers.

For more information

To learn more about IBM Healthcare and Life Science Solutions and IBM Business Partners, visit **ibm.com**/industries/lifescience or contact an IBM Healthcare and Life Sciences specialist at LS@us.ibm.com.

To learn more about Accelrys, visit the Accelrys Web site at **www.accelarys.com**, Or contact an Accelrys specialist via the online information request form at **www.accelerys.com/about/enquiry.php**.

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