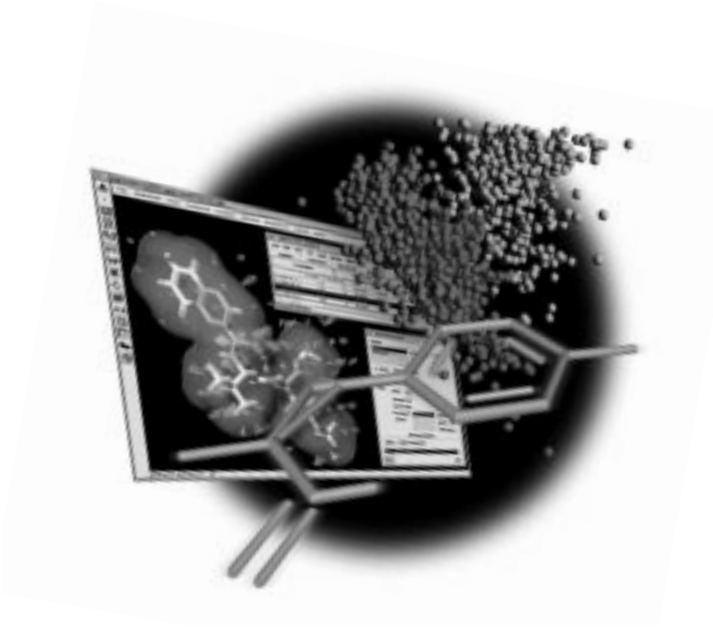
SiliconGraphics
Computer Systems

Chemical and Biological Information Management



Building the Scientific Enterprise

Virtual Laboratories: The New R&D Workflow

Sophisticated computer-controlled robotic and simulation processes are revolutionizing today's lab environments. To be effectively exploited, the associated explosion of chemical and biological data must be distributed, accessed, and analyzed. Meeting this challenge is critical to your success. Effective scientific information management solutions require more than a combination of software and hardware—they require collaboration between a technology provider and your research team. Silicon Graphics allows you to get the most from your data by offering high-performance servers, strong relationships with the premier software companies, and a desire to help create the most productive chemical and biological information management environment for your organization.

Powerful Tools for Scientific Information Management

Silicon Graphics, together with the industry's leading application software vendors, helps you build and deploy a robust scientific computing environment. Silicon Graphics' alliances have produced an unmatched range of scientific information management solutions. Origin™ servers offer the leading commercially populated and public domain databases and the software products you need to effectively input, access, search, manage, and analyze 2D and 3D chemical structural and biological property data. Application software providers deliver tools for Origin servers that also let you design, build, and optimize combinatorial chemistry libraries and analyze high-throughput screening results. These data analysis and data mining tools, combined with Silicon Graphics MineSet software, empower scientists and discovery teams to quickly make research decisions.

A Sampling of Supported Software

Application Vendors

MDL: ISIS/HOST™, MDL SCREEN™, Central Library™, Chemscape™

Daylight Chemical Information Systems: Daylight™,Thor Merlin

Molecular Simulations, Inc.: Catalyst™,C2™, WebLab™ Diversity Explorer™, MedChem Explorer™

Oxford Molecular Group: RS^3™ Discovery, DIVA™

Chemical Design: Chem-X

Tripos, Inc.: UNITY™, Legion™, Selector™, ChemEnlighten™, ChemSpace™

RDBMS Vendors

Oracle

Informix

Sybase

Web Servers

Netscape® Enterprise Server

Apache

CORBA Libraries

IONA

VISIGENICS

DCOM

Data Mining and Visualization

Silicon Graphics® MineSet™

Datasheet

The Compute Cornerstone

Origin servers encourage efficiency in all areas of your organization, shortening the time for discovery research and improving the probability of getting products into the research and development pipeline. Researchers benefit from superior computational and I/O performance and from application software that has been parallelized to keep search times down as data volumes and usage go up. Origin servers uniquely meet all of the requirements for every scientific information management application:

- Scalable systems—Origin servers span the range of your needs. From Origin200™ for departmental chemical information systems to Origin2000™ for organization-wide systems, Silicon Graphics systems fit a broad variety of search and database requirements and can grow to handle larger tasks, larger databases, and more users
- 64-bit system architectures—databases demand a high-throughput platform and a memory addressing scheme that optimizes searches. The 64-bit hardware and operating system from Silicon Graphics streamline data handling. They also provide a scalable and robust I/O system that enhances overall performance when using the large databases typical in combinatorial chemistry
- High availability—Silicon Graphics IRIS FailSafe™ environment lets you protect critical information and ensures that global research teams are not affected by any system or network disruptions
- Web serving technology—a strong suite of high-performance Silicon Graphics Web products keeps researchers linked to the worldwide community and ensures effective decision making within your organization

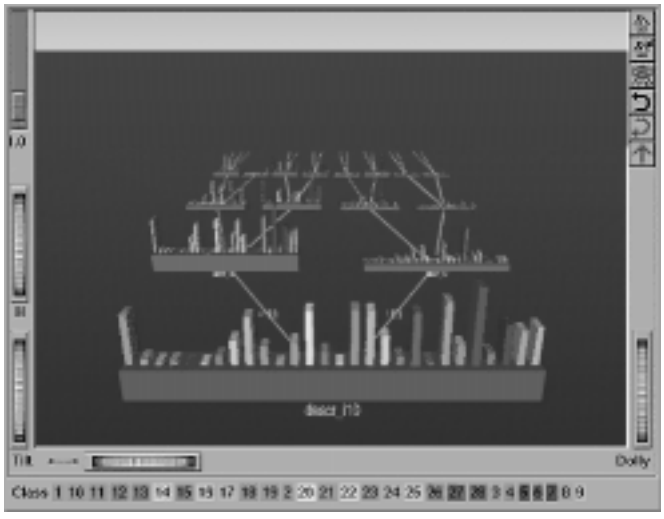
Plenty of headroom across the entire system—I/O, processors, and memory—means that Silicon Graphics systems can accommodate large 2D or 3D data sets serving large work groups and still deliver exceptional system response and interactivity. Upgrades make expansion affordable and allow you to grow system capacity as your needs expand.

Silicon Graphics and Tripos, Inc.

Needs: Pharmaceutical and biotech research organizations rely on virtual laboratory solutions to speed the search for appropriate target compounds, allowing for quick comparison of the results from many reagent tests. Chemists also require analysis tools to accurately predict compound classes based on a set of compound descriptors.

Solution: Tripos built a virtual combinatorial chemistry database, based on the company's ChemSpace technology, which offers chemists information about more than 180 billion compounds. Silicon Graphics servers host the database and Silicon Graphics workstations provide the graphics and data navigation technology needed to transform the data into intuitive 3D representations. Tripos used Silicon Graphics MineSet data mining and visualization software to segment the results data set to identify the best descriptors for predicting correct classes for each compound. The MineSet Tree Visualizer offers at-a-glance results of the compound similarity based on various reagents.

Benefits: The Tripos/Silicon Graphics solution delivers high-throughput data screening capabilities, returning hundreds of thousands to millions of data hits for search operations. The optimized screening means that researchers rapidly uncover insights from the Tripos data. The 3D visualizations of MineSet give informative views of all data, a unique visualization capability for such large data sets. The power of the information in the virtual library can be effectively used in the discovery process.



In the image above, the MineSet Decision Tree Classifier was used to create a segmentation of the Virtual Combinatorial Chemistry data set, based on values of the different descriptors, to determine what priority the descriptors have in predicting the class to which a compound belongs.

WebLab MedChem Explorer from Molecular Simulations Inc. provides access to powerful Silicon Graphics Origin servers for performing lead identification and optimization, including database searching, property calculations, conformer generation, molecular alignment, and pharmacophore model generation.

Silicon Graphics and Molecular Simulations Inc. (MSI)

Needs: Intuitive tools for medicinal chemists to search chemical databases, develop predictive models, and prioritize compound synthesis; intuitive tools for synthetic chemists to design, build, and analyze combinatorial libraries.

Solution: MSI offers a suite of software tools—MedChem Explorer™ and Diversity Explorer™—built upon MSI's WebLab™, a client-server environment running on Silicon Graphics servers. Both tools provide a straightforward, single-task focus for simulated experiments. WebLab unifies an easy-to-use Web browser interface with validated computer simulations. MedChem Explorer combines the strengths of cheminformatics and molecular modeling tools for the medicinal chemist, and Diversity Explorer combines molecular modeling and analysis tools for the synthetic chemist.

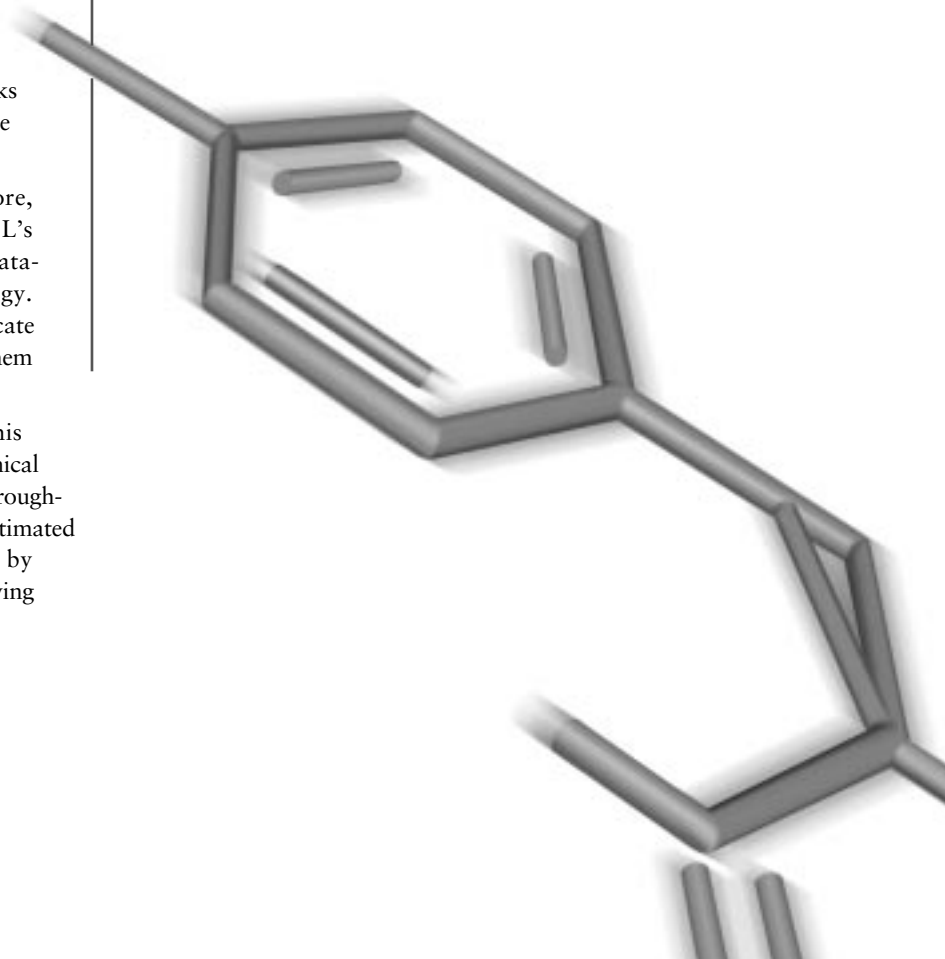
Benefits: The combination of Web browser clients with validated molecular modeling software on powerful Silicon Graphics servers provides medicinal chemists with the ability to quickly make decisions and prioritize the synthesis of lead compounds. Synthetic chemists get the autonomy they need to easily assemble a library based simply upon reagents and the reactions that they undergo.

Silicon Graphics and MDL at Affymax

Needs: Easy-to-use tools for specifying, locating, ordering, and registering chemical building blocks that help bench chemists prepare to synthesize compounds.

Solution: Silicon Graphics servers deliver ChemStore, an innovative Web-based system utilizing MDL's Chemscape software and databases, Oracle databases, and Netscape Enterprise Web technology. The online store allows chemists to quickly locate chemicals within the company before ordering them from vendors.

Benefits: Used extensively by Affymax chemists, this system has eliminated tedious scanning for chemical compounds in catalogs and day-long searches throughout other company labs. ChemStore saved an estimated $91,000 in its first six months of deployment by speeding the retrieval of compounds and improving the tracking of every chemical purchase.



Solutions
At a Glance

	O2™	OCTANE™	ONYX2™ SERIES	ORIGIN200™	ORIGIN2000™
					
	PERSONAL WORKSTATION	POWER WORKSTATION	VISUAL SUPERCOMPUTER	SERVER	SCALABLE SERVER
CHEMICAL DATABASES; COMBINATORIAL CHEMISTRY	Statistical analysis, 2D and 3D desktop, chemical database access	2D and 3D structural databases, combinatorial chemistry	Scalable simulation, 2D and 3D structural database serving, combinatorial chemistry	Departmental chemical registration system, combinatorial chemistry	Scalable 2D and 3D structural database serving, combinatorial chemistry
INTRANET AND INTERNET	2D and 3D desktop access, personal Web server	2D and 3D desktop access, personal Web server	Visual Web serving	Interactive information exchange, media serving, Web serving	Interactive information exchange, media serving, Web serving
DECISION-SUPPORT AND DATA VISUALIZATION	Visual data mining	Visual and analytic data mining	Visual and analytic data mining	Small to medium data warehousing and analytic data mining	Very large data warehousing and analytic data mining
	To obtain more product, application, and solution information, visit our Web site at *www.sgi.com/chembio*.				

The Silicon Graphics Winning Combination

The scalable performance and large data-handling capabilities of Silicon Graphics servers have attracted the industry's premier databases and solutions for combinatorial chemistry, high-throughput screening, and chemical databases. Choosing a Silicon Graphics foundation for your research and development team ensures reliable access to the latest software, tools, and databases that help speed your projects to completion.

Silicon Graphics Origin servers flexibly address all of your scientific computing requirements. Dedicate a server to a key database, and speed access times for your entire team of researchers. Or combine previously separated phases of discovery research—design, synthesis, and informatics—on the same system for an optimized workflow within your organization. The complete range of application software tuned for Silicon Graphics systems lets you modify configurations to fit your projects at hand, resulting in the most return for your compute investments.

Silicon Graphics' in-house expertise underscores the company's commitment to your business. With an international team of chemists and biologists, Silicon Graphics can address your unique project needs and help optimize a solution for your chemical information management system.

Front Cover Image:
Left: *Image generated by SYBYL and UNITY from Tripos.* **Right:** *Partial image from Molecular Simulations, Inc. WebLab MedChem Explorer screen. Molecular image courtesy of Affymax Research Institute.*

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