

Visualization in Drug Discovery: The Way of the Future

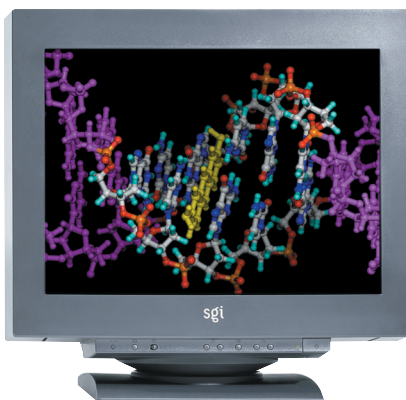
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The pharmaceutical drug discovery process is in the beginning of a revolution: visualization is being used to transform large data sets into 3D graphical images, enabling internationally distributed groups of users—in immersive, theater-like environments—to interact with and manipulate those images in real time.

These technologies have been demonstrated to enhance collaboration, so that more effective decisions can be made more rapidly.

Discovering new drugs involves the efforts of many highly motivated researchers working across a range of disciplines toward a common goal—to bring a new therapeutic drug to the market as soon as possible. This process is often fragmented, because so many different departments within an organization are involved in the development of a new drug. Three-dimensional visualization technology—the process of visually representing abstract scientific data as images, aiding in understanding the significance of the data—is helping pharmaceutical companies to speed up the drug discovery process significantly.

Many innovative pharmaceutical companies are now using visualization centers in which scientists can, in group settings, study, interact with, and manipulate large visual data sets projected on screens. Visualization acts as a catalyst in the generation of new drug design ideas and empowers both project teamwork and stimulating discussions among chemists, biologists, and computational chemists. The return on investment (ROI) is twofold: more effective use of collective knowledge through better interactions between scientists and the quicker production of actionable decisions by consensus.



A complementary technological advance set to revolutionize the drug discovery process is Visual Area Networking. This concept, introduced by SGI in early 2002, takes collaborative visualization one step further: end users don't need to be in a visualization center to access the data. Instead, a single source of data can be computed and processed for visualization on a single system, but the visual output can be accessed remotely on any device—PC, laptop, tablet PC—anywhere in the world via a simple Internet connection.

The ROI for implementing collaborative visualization in drug discovery environments has demonstrated a significant competitive advantage to organizations possessing this infrastructure. A conservative estimate of time saved on the discovery processes is 2% and, when calculated against the average cost to develop a drug and the projected revenue per year of a drug, estimates of ROI for implementing visualization can be easily calculated. Using this technique, organizations can conservatively expect to save approximately \$80 million per drug by implementing a collaborative visualization environment for their researchers.

As the industry enters into what could be termed a “post-genomic period,” involving ever-increasing high-performance computing and collaborative visualization needs, these technologies are solutions that can meet the challenges facing the industry today and tomorrow. Pharmaceutical companies need to be able to evaluate as many potential drug molecules as possible in the shortest time. They also need to be able to recognize dead-ends as early as possible so that they can redirect resources to the best leads. Visualization technologies will help researchers worldwide achieve these objectives in a more efficient and cost-effective way.

For further information about the SGI concept of Visual Area Networking, visit www.sgi.com/visualization/van, and for details about SGI's involvement in the life and chemical sciences, visit www.sgi.com/go/chembio.