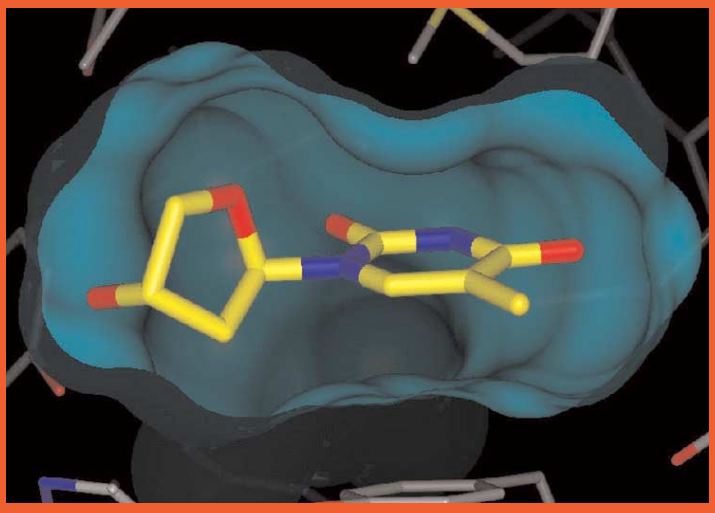
Success Story

Empowering Drug Discovery Teamwork

Discovery Teams at Janssen Pharmaceutica Are Using SGI® Technologies to Innovate Their Research

Therapeutic drug compounds are not discovered by coincidence; they are created. In 1953 Dr. Paul Janssen began small-scale chemical and pharmacological research in his drive to create innovative therapeutic compounds. Today, Janssen Pharmaceutica is a world-class leader representing the highest standards in quality—in the products it produces and in the employees who produce them.

To remain on the leading edge requires innovation. Janssen Pharmaceutica sets the pace for drug discovery using an SGI® Reality Center™ facility powered by SGI visualization technologies. The Reality Center environment enables Janssen Pharmaceutica to provide exactly the technology its project teams need to maximize their ability to incorporate structure-based drug design into the drug discovery process. First-rate research is ongoing to discover novel therapeutic molecules targeting cancer, Alzheimer's disease, depression, schizophrenia, metabolic diseases, and gastrointestinal disorders.



Drug Discovery

At Janssen Pharmaceutica hundreds of new molecules are being synthesized each day. However, not all of these molecules will later become novel therapeutic drugs. Only one compound in 5,000 will reach the final stage of becoming a useful therapeutic drug that may help millions of patients, a process that takes more than 10 years of labor-intensive, interdisciplinary research.

The Reality Center facility helps Janssen Pharmaceutica to significantly increase the speed and efficiency of the drug discovery process. To a large extent it acts as a catalyst in the generation of new ideas in drug design and empowers project teamwork and stimulating discussions among chemists, biologists, and computational chemists. Using the high-throughput screening technologies afforded by SGI Reality Center, Janssen Pharmaceutica researchers looking for molecules with the desired therapeutic profile are now able to conduct extensive tests on up to 100,000 chemical compounds a day.

Innovation

Innovative research at Janssen Pharmaceutica has always been the driving force behind its continuing success. In the quest to understand the relationship behind therapeutic effects and chemistry, powerful computer algorithms are now used to simulate and analyze the binding between drug and disease protein. Janssen Pharmaceutica researchers are using state-of-the-art SGI high-performance computing technologies to investigate the interaction of candidate drug molecules with their target receptors and are using this information to further develop drug compounds that have optimal action profiles with fewer adverse effects.

"The most significant benefit of the Reality Center facility is the way researchers interact with the system."
—Hans De Winter, Senior Scientist
Janssen Pharmaceutica, Belgium

The Silicon Graphics® Octane2™ is configured with:

- Two R12000™ processors at 400 MHz
- 2GB of main memory
- V12 VPro™ graphics system
- A tiltable, rear-projected BARCO™ BARON® display table
- Active stereoscopic implementation

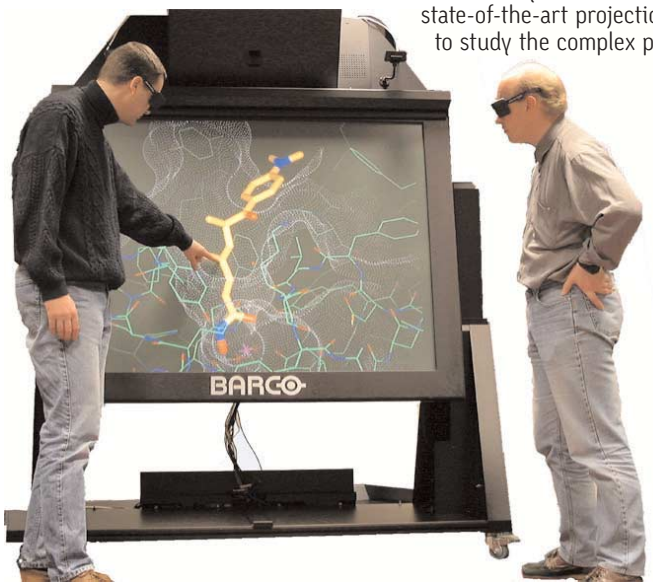
Teamwork

The process of discovering new drugs is a complicated one. It involves the cooperative efforts of many highly motivated researchers aiming toward a common goal: to bring a new therapeutic molecule to the patient as soon as possible. Project teams, with the help of visualization technologies, are empowering the research within Janssen Pharmaceutica.

According to Hans De Winter, Senior Scientist, Janssen Pharmaceutica,"Typically, Janssen Pharmaceutica researchers from pharmacology, biology, chemistry, and molecular modeling departments interact with the Reality Center environment in small, flexible teams of up to 10 people. The most significant benefit of the Reality Center facility is the way researchers interact with the system. Because SGI visualization technology enables the projection of large, realistic, and 'human-sized' images of drugs located in protein pockets, researchers are able to become completely immersed within the target protein and, as such, obtain a realistic feeling about the important molecular functionalities and how to elaborate further on them."

Visualization

As data output increases and becomes more and-more complex, cutting-edge visualization technologies are having an enormous impact on drug discovery project teams. The Janssen Pharmaceutica Reality Center facility is a state-of-the-art projection facility used to study the complex patterns of interaction between therapeutic lead compounds and their disease targets. Sophisticated visualization of 3D protein cavities with bound inhibitors serves as a catalyst for the generation of new ideas for finding novel therapeutics. Realistic in-depth projections are stimulating researchers on the project teams to exchange their ideas and to discuss alternative chemical modifications in the fast-moving field of pharmaceutical research.



For the researchers at Janssen Pharmaceutica, it has become the norm to use 3D projection systems powered by cutting-edge, high-performance SGI computing systems as powerful communication tools. This novel technology is driving the search for better medicines into a new era.

The heart of the Janssen Pharmaceutica Reality Center facility is the Silicon Graphics® Octane2™ V12 VPro™ graphics computer, a small-scale, high-performance option in a range of increasingly powerful visualization technology solutions.

A specially designed multimedia room has been made available for Reality Center sessions. Applications can be driven either from a console close to the graphics computer (with a dedicated stereo monitor) or directly from the display table, which is also equipped with a keyboard, a mouse, and an additional dial and button box.

SGI Professional Services

SGI Professional Services expertise in Reality Center installation and integration played a significant role in helping tailor a visualization technology solution that advanced Janssen Pharmaceutica's commitment to leading-edge research. In addition, SGI Professional Services collaborated with Janssen researchers to ensure that the computing solution chosen for the system would optimize their research efforts.

Optimizing the Future

Advanced visualization and high-performance computing technology solutions from SGI enable collaborative research efforts, expedite insights into complex problems, and streamline the drug discovery process. From advanced 3D modeling and simulation to digital prototyping and group visualization, SGI transforms product development processes, thereby enabling the pharmaceutical industry to develop optimized drug compounds in less time and to reduce the time to market for new therapies.

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