



## POWERWULF CLUSTERS: COMPUTATIONAL CHEMISTRY

### CASE STUDY

PSSC LABS POWERWULF CLUSTERS SUCCESSFUL  
ACCELERATE PHARMACEUTICAL RESEARCH.

#### PROFILE

Aventis Pharmaceutical

#### CHALLENGE

It is generally accepted that it takes about ten to fifteen years from the time that research and development of a drug is started to when that drug is brought to market. Frequently, for various reasons, the drugs will never become commercially viable so any reduction in time spent in development results in cost savings to the company. One glaring is insufficient computing power. Anil Nair, Senior Associate Scientist at Aventis agreed, "Previously, researchers were limited by the speed with which 'virtual screening' of small molecule libraries was performed. With the AMD processor-based cluster, I can utilize parallel processing to work through myriad possibilities to eliminate the bad ones and find the best choice. We can perform a 'virtual screen' on 10,000 or more small molecules each day."



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### CASE STUDY CONTINUED

#### SOLUTION

PowerWulf Clusters are helping accelerate pharmaceutical research for Aventis, the prescription-drug and vaccine company, best known as the makers of Allegra. The successful implementation of this custom PowerWulf Cluster solution is evidence that the investment in technology integration is a key factor in reducing product cycles and bringing new and helpful drugs to the marketplace.

"At PSSC Labs, we've recognized how critical it is for pharmaceutical firms to reduce the time and money that they spend on research. After building custom PowerWulf Clusters for firms like Aventis and Concurrent Pharmaceuticals, we understand the specific research needs of the pharmaceutical industry and tailor our machines to meet their requirements," said Alex Lesser, Vice President of PSSC Labs.

#### IMPACT

The PSSC Labs PowerWulf Cluster is tasked with quickly identifying small molecules that will either inhibit or activate a targeted protein. Once identified, Aventis can work to alter the functions of these proteins. Such research is vital to treating diseases like cancer and diabetes. Sorting through the vast mathematical possibilities of molecular research is closely tied to the performance of the processor's floating-point engine. "There's no question that one of the great strengths of this cluster is its ability to crunch numbers," said Lesser "and we've found that this is invaluable to our pharmaceutical and biotech clients in terms of return-on-investment."

Nair is eager to build upon the current increase in productivity by adding more nodes to his system, saying he plans to double its size – with expectations of doubling researchers' productivity – in the coming year. "We're excited about the potential of this very powerful new tool," he says. "It's making a substantial difference in the way we do research."