IN 60 MINUTES
SCHRÖDINGER CAN TEST 16 MILLION MOLECULES, SO PHARMACEUTICAL RESEARCHERS CAN MAKE BREAKTHROUGHS SOONER

"For years, pharmaceutical companies have been scaling up staffing resources via contract research organizations. Now, thanks to high performance computing in the Amazon Web Services cloud, it's incredibly simple and cost-effective to scale their compute resources in a similar way."

—Scott Becker, VP of Enterprise Products, Schrödinger

ON-DEMAND SCALABILITY:

1 to 50,000

INTEL® XEON® PROCESSORS

ACCELERATING PHARMACEUTICAL BREAKTHROUGHS WITH HIGH PERFORMANCE CLOUD COMPUTING

Research teams can spend nearly a decade looking for new biological targets. Then years more creating and testing new molecules that offer improved ways to fight the world's viruses, bacteria, and diseases.

Schrödinger software is helping researchers drastically decrease those timelines. The company's Glide* solution virtually screens billions of molecules in a fraction of the time it would take to test them in labs. But the solution requires an immense amount of computing power.

RESEARCH AT 16 MILLION STEPS PER HOUR

A team of cancer researchers recently came to Schrödinger with a drug concept and a list of tens of millions of molecules. They also had a tight deadline, a fixed budget, and strict security and compliance requirements.

That's when Schrödinger turned to Amazon Web Services. Without any up-front investment in infrastructure, Schrödinger leveraged software from AWS partner Cycle Computing (cyclecomputing.com) to provision a fully secured cluster of 50,000 cores, powered by the Intel® Xeon® processor E5 family.

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This configuration enabled the team to run 16 million molecular simulations an hour. These simulations, which would have tied up Schrödinger's limited number of in-house servers for weeks, took just eight hours. Best of all, the researchers now had a manageable list of 1,000 molecules ready to take into the next phase of lab testing.

THE COST-EFFECTIVE POWER OF ON-DEMAND SUPERCOMPUTING

When the simulation was complete, Schrödinger was able to switch off the 50,000 cores and stop incurring charges immediately. When the next project rolls in, the company will be able to quickly spin up the perfect amount of resources to fit the requirement—again without any up-front investment.

Having this large-scale, powerful infrastructure available on demand gives Schrödinger an amazing amount of business agility. Not only is the company able to process existing simulations in less time, but it can also take on more concurrent projects, driving more scale and value for its customers.

For more information on Schrödinger projects, go to schrodinger.com.

GET STARTED FOR FREE ›

ON-DEMAND SUPERCOMPUTING SPEED:

16 million molecule simulations an hour

"WE CAN SUPPORT 200 TIMES THE PROJECTS NOW VERSUS WHEN WE RELIED ON JUST OUR OWN SERVERS."

—Scott Becker

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