Chemotargets unleashes creative data processing

The biotechnology company relies on the HP Z8 G5 workstation to perform complex data processing faster and with many more simulations performed at the same time

Chemotargets



INDUSTRY:
Biotechnology

COUNTRY:
Spain

Objectives

Chemotargets is a pioneer in AI-led computational approach to assessing drug safety, efficacy and designing novel molecules for new medicines.

The company recently made a transition from a software business to biotech with its own drug discovery pipeline. But with its growth and ambitions came the need for more computational power to manipulate complex sets of data.

"The amount of data we handle has increased tenfold and the algorithms applied to those datasets have become more complex," said Dr. Scott Boyer, CEO of Chemotargets.

"The computations in the cloud became expensive, slow and burdensome. Our objective was to bring as much computation in-house and gain more flexibility in terms of the GPUs (graphics processing units) and the CPUs (central processing units) for various tasks."

> "We do exactly what we need to do, in the order we need to do it in, instead of spreading it in a dozen different directions and compiling the results afterwards."
>
> Dr. Scott Boyer
> CEO, Chemotargets

Solution at a glance

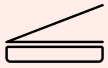
HP Services

Z8 G5 & Z8 Fury G5

Ultra-Fast Memory Configurations up to 2 TB DDR5

Intel® Xeon® W9 Processor up to 56 Cores

Up to 4 High-End GPUs



From 3 weeks to 2 days for molecule scans



Performance and speed at a lower cost

Approach

Accessing resources in the cloud is expensive for small companies, which means running jobs meant for GPUs on CPUs. “But running them simultaneously for various tasks means that you can have a lot of parallel threads operating at the same time, complementing each other,” said Boyer.

The company decided to try out an HP Z8 G5 workstation to save on processing time and cloud computation costs. “We were a little bit agnostic about compute resources, but we were offered a demo machine by the HP Data Science team to try out and its specifications fit the way we work,” commented Boyer. “Fast computation and the large memory allow for the management of large datasets. And we didn’t have to prioritize the work as much. The machine had the capacity to take care of nearly every one.”

But most importantly, more creative work is now possible. “We’ve done a lot more exploration with methods, approaches and datasets than we would have in the past. It broadens the number of ideas that could be explored without having to worry as much about the cost.”

Business Outcomes

The time to make calculations scanning the surface of a single molecule is down from three weeks to two days. “We do exactly what we need to do, in the order we need to do it, instead of spreading it in a dozen different directions, individual networks and the cloud, and then compiling the results afterwards,” said Boyer.

The capacity to run multiple tests and simulations simultaneously contributes to efficiency and creative problem solving. “But most noticeable is the unexpected level of happiness among our staff. They even had plans to network everybody’s laptops together to gain capacity. It’s most satisfying to know that we, together with HP, made their life easier.”

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