

AZothBio Accelerates New Drug Discovery Using Deep Learning on Rescale

Case Study



Headquarters: Seoul, Korea
Industry: Bio-Tech, Pharmaceuticals
Founded: 2016

Challenge & Solution

In order to accelerate lead identification for new therapies, AZothBio needed a flexible, scalable, and performant compute that was simple to deploy and cost effective due to their capital and people constraints as a new venture. Rescale's platform for intelligent computing was able to quickly onboard and optimize their applications for speed and cost-performance.

"Through Rescale, we were able to draw results more than 2x faster than our existing workflow, which helped us make better business decisions."

Jerry Maeng
 Managing Director, AZothBio

Software Deployed on Rescale:



AutoDock Vina



In-House Python
 AI Codes

From Startup to World-Class Bio-Pharmaceutical Company

The team of researchers, scientists, and engineers at AZothBio bring rich experience from their backgrounds in life sciences, biotechnologies, and pharmaceuticals. Their mission is to combine their expertise to catalyze new drug discovery and bring more competitive products to more patients. When conducting their research and development, AZothBio uses digital tools and proprietary artificial intelligence logic to uncover new therapies and drug candidates. These techniques require significant high performance computing (HPC) resources to handle high fidelity simulations.

When AZothBio's compute demands exceeded the capabilities of their on-premises hardware, they sought a solution from Rescale that could support their complex and custom applications in a way that is simple, scalable, and allowed them to focus on what they do best: cutting-edge R&D innovation. In order to simulate large-scale algorithms in the cloud, understanding not only the R&D challenges but also cloud infrastructure, HPC, and configurations is essential. To save critical time and productivity, AZothBio adopted the Rescale platform to transform their digital capabilities.

Transforming R&D Capabilities to Meet Urgent Public Health Needs

AZothBio first collaborated with Rescale through the Tech Against COVID-19 program by using Rescale's cloud HPC environment which allowed AZothBio to easily onboard their software and use their methodology to conduct COVID-19 research. Using Rescale's end-to-end HPC-as-a-Service workflows, AZothBio was able to quickly identify the best infrastructure on AWS (also a sponsor for the Tech Against COVID-19 initiative) to run their workloads using hardware with the best performance profile based on their unique software needs. Through this program, AZothBio initiated a project to discover immunoreactive substances targeting the infection of the coronavirus and quickly expanded to other projects.



Pictured Above: Jerry Maeng (Left), Dr. Hyejin Park (Right)

Because the bio-pharmaceutical industry is highly competitive with limited resources, a high degree of focus and efficiency is required to succeed. AZothBio, a lean startup but quickly growing in the biomedical field, needed a solution to enhance the agility of their R&D operations. Using the Rescale platform, AZothBio was able to create a research system for selecting drug candidates with efficient cost-performance while accelerating lead identification through massive data analysis and predictive simulation using their own proprietary deep learning-based algorithms in ways not possible with traditional methods.

AZothBio's proprietary epitope prediction AI model uses deep learning processes, and analyzes the biological data related to antigen/antibody reactions to predict peptide sequences that activate the immune response. The combination of the AI model and genome analytics widens the possibilities for developing immunotherapeutic drugs and vaccines. However, as they scaled up multiple areas of research their on-premises compute environment could not support the capacity and complexity of their tools, and it would be time and cost prohibitive to rebuild them in-house. Through Rescale, the team was able to access pre-installed software and the best-fit GPU hardware (NVIDIA V100 cloud instances) to successfully run their epitope AI models and expedite their other efforts in genome and peptide discovery research from 5 days to within 24 hours per analysis.

Harnessing Platforms to Power Modern Innovation

Having the right platforms for innovation can accelerate the prediction and identification of lead drug and therapy candidates. "Rescale was immediately deployable and offers an easy-to-use environment. Previously, it was a significant burden on our side to set up GPUs and we are happy to now have Rescale to drive critical analysis and reduce the risks of cost and delays," said Managing Director of AZothBio, Jerry Maeng. They plan to continue to partner with Rescale to deploy new AI models for lead identification to become a global leader in bio-pharmaceutical innovation.



Rescale optimizes 850+ HPC applications on any hybrid cloud architecture

SPECIALIZED GPU HARDWARE
FOR AI/ML WORKLOADS



- » Volta V100
- » Tesla P100, M60, K80
- » NVLink

"As a researcher, I don't have much experience in IT, so I was nervous migrating our HPC to the cloud. But Rescale's user-friendly platform did not require expertise in IT or HPC. Also, Rescale understands both HPC and R&D fields, which provides us crucial support and lets us focus solely on R&D."

- Dr. Hyejin Park, Director AI Research Institute, AZothBio

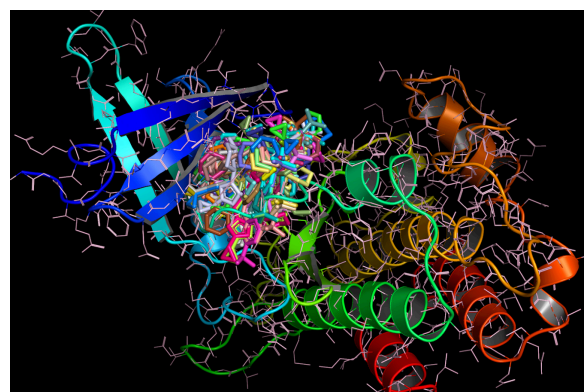
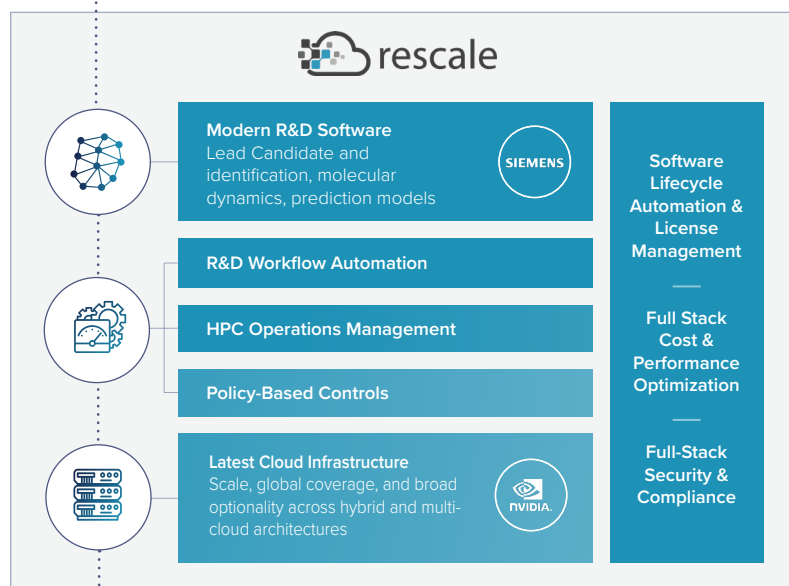


Rescale Unifies Best-in-Class Tools For Bio-Pharmaceutical Digital R&D



Digital R&D Objectives

- » Accelerate Lead Identification
- » Reduce IT Burden
- » Increase Model Fidelity & Scale
- » Improve Collaboration



Featured Platform Software: AZothBio AiDL

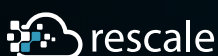
AZothBio's proprietary in-house platform, AiDL, is used to generate an ensemble of 3D components to accurately create the visualization necessary to confirm that the drug is binding to the target protein. By using artificial intelligence and deep learning, AiDL enables rapid and efficient screening by drastically reducing the initial stage of drug discovery.

For more information on AiDL visit:
azothbio.com/new/eng/main/main.php



Strategic Business Outcomes

- » Accelerated Time-to-Market
- » End-to-End Automation
- » Improved Quality & Competitiveness
- » Increased R&D Productivity



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About Rescale

Rescale helps organizations accelerate science and engineering breakthroughs by eliminating complexity. From supersonic jets to personalized medicine, industry leaders accelerate new product innovations with unprecedented speed and efficiency with the Rescale Platform - a solution for intelligent full-stack automation for big compute and R&D collaboration on hybrid cloud. Rescale enables IT leaders to deliver high performance computing-as-a-service, with software automation on a hybrid-cloud control plane with security, architecture, and financial controls. Learn how you can modernize high performance computing at Rescale.com