Optimize drug discovery pipelines with NVIDIA BioNeMo

In collaboration with: rescale

Train, develop, and deploy generative AI models for drug discovery applications running on Rescale with AWS and NVIDIA

Rescale's high performance computing (HPC) platform running on Amazon Web Services (AWS) provides on-demand access to the latest software and hardware for drug discovery workloads. Scale and run computationally intensive workloads and deploy AI-enabled drug discovery applications on more than 1000 pre-installed and fine-tuned commercial and open-source software such as GROMACS and LAMMPS.

Rescale makes building an advanced and innovative drug discovery pipeline with generative AI simple. It pairs with NVIDIA BioNeMo using Amazon Elastic Compute Cloud (Amazon EC2) instances, powered by NVIDIA GPUs, and accelerates the process with pre-loaded, ready-to-use templates that access custom data directly from AWS services such as Amazon EC2, Amazon Elastic Block Store (Amazon EBS), or Amazon FSx for Lustre.

NVIDIA BioNeMo is a fast and easy way to build and integrate state-of-the-art generative AI applications across the entire drug discovery pipeline. It includes:

- Services to develop, customize, and deploy foundation models for drug discovery
- A collection of pretrained biomolecular AI models for protein structure prediction, protein sequence generation, molecular optimization, generative chemistry, docking prediction, and more
- Easy-to-access APIs for inference and customization

Using Rescale, BioNeMo seamlessly scales with dataset sizes, model sizes, and training tasks, and reduces time and cost for model development. To run efficiently BioNeMo needs access to large data storage and high performance, networked GPUs. Rescale manages this HPC environment on AWS with complete administrative control, so customers have the power of AWS infrastructure without worrying about performance, security, or budgets.

NVIDIA BioNeMo + AWS + Rescale

Generative AI platform for drug discovery

AI models
Predicting protein and small-molecule properties (ESM-1, ESM-2, MegaMolBART, MoFlow), protein generation (ProtGPT2), pose prediction (DiffDock), and 3D protein structure prediction (OpenFold, AphaFold2, ESMFold).

AI workflows
3D protein structure prediction, de novo design, virtual screening, docking, and property prediction.

Flexible and secure cloud services

Available in almost every major region where AWS operates, Rescale on AWS offers a turnkey HPC solution with virtually limitless scale and flexibility.

Deploy a complete HPC solution on AWS 20 times faster with Rescale to accelerate the time-to-value backed by AWS Support.

Fully automated for life sciences R&D

1000+ leading HPC software options for life sciences, pre-installed, fine-tuned, and ready to deploy.

AI workflows
Training pipelines, data selling: labeling, inference prediction, results visualization, simulation validation.

Accelerate the journey to AI-powered drug discovery today ›