



PIONEERING THE FUTURE OF LIFE SCIENCES WITH AI

Supercharge a new era of silico drug discovery



Today's organizations are adopting an AI platform to achieve faster results:

- Predicting chemical properties at experimental accuracy
- High-throughput virtual sequencing to evaluate billions of molecules
- Generating 3D models in near-atomic detail to gauge the effectiveness of new drugs
- Unprecedented acceleration to primary, secondary, and tertiary analysis of genomic data
- Protein structure prediction from genome sequence using deep learning techniques
- Real-time single cell RNA data visualization and interpretation

A NEW AGE OF LIFE SCIENCES

Artificial intelligence (AI) is transforming the future of drug discovery. Accelerated computing with AI has launched an entirely new paradigm that is streamlining the investigation, assessment, and creation of new drugs and therapies. These capabilities can be applied to evidence-based treatments, disease prediction, and prevention, bringing tailored therapies into widespread use. However, the exponential growth of life sciences data has put pressure on organizations to evolve. By 2025, data volumes are expected to reach 200 zettabytes. Although this data holds the potential to enable the next scientific breakthrough, issues including computational bottlenecks, limited access to mission-critical information, and poor predictive validity are major roadblocks on the path to discovery.

With legacy technologies running data analysis, the industry has experienced a decrease in workplace productivity as well as an increase in research and development (R&D) costs. R&D spending is expected to rise from \$83 billion in 2019 to roughly \$203.9 billion by 2024. Despite the excess spending, the industry is projected to see a decline in drug discovery with fewer new drugs brought to market. At the same time, human genome data analysis requirements are growing at an unprecedented rate. With over two million genomes to be sequenced by 2025, the need for processing and analysis will make genomics one of the most demanding data domains in existence. Organizations are racing to adopt technologies that will provide greater precision and predictability to help them boost productivity in a thriving digital workplace and overcome their greatest challenges.

Today, life sciences organizations are unlocking more value from massive amounts of data with AI. Cutting-edge technologies can dramatically shorten the rigorous and time-consuming process of finding, testing, and approving new drugs by helping organizations to understand disease biology at the molecular level and accelerate better therapeutic outcomes.

Organizations that partner with HPE and NVIDIA are revolutionizing life sciences research with better performance and faster results:

- Screening 2 billion compounds 33x faster (one day versus three months)
- Screening 10 million drugs 100x faster (eight minutes versus 240 days)
- 76x improvement in throughput performance for WGS

AI-POWERED LIFE SCIENCES APPLICATIONS

Bringing new drugs to market takes 10 to 15 years from drug discovery, pre-clinical studies, clinical trials, and FDA review to finally, large-scale manufacturing. Few of the compounds initially identified will become an FDA-approved drug that goes into distribution. AI is helping to make this a predictive process with greater intelligence, higher productivity, and lower costs across all key workflows.

The more compounds an organization can identify and screen, the more drugs it can discover. It can take an enormous amount of lab time to test which drug out of thousands will be safe and effective. AI accelerates virtually every computational chemistry code to speed up and reduce the costs of R&D, enable more accurate findings, and increase the likelihood of drug program success. Using information-dense data from cutting-edge analytics instruments such as cryo-electron microscopes (cryo-EM), organizations are leveraging more of their data to derive value from their drug discovery workflows. Many organizations are reaping the benefits of the latest cryo-EM technology to produce better drugs in less time that target a wider range of debilitating diseases.

Next-generation sequencing (NGS) has revolutionized genomics and fueled the evolution of drug discovery and treatment efforts worldwide. Due to the rapid growth of sequencing workloads, NGS requires innovative AI tools to meet the increasing demand for processing and analysis. The integration of these capabilities drives remarkable improvements in translational life sciences research by determining the relationship between genotypes. Many of today's researchers are modeling the human genome against infectious diseases to develop tailored drugs and therapies. Life sciences research institutions are analyzing petabytes of data to pinpoint the differences in people's genes, environments, and lifestyles to aid in disease prevention. In pharmaceutical and biotech, companies are using AI to accelerate drug and vaccine discovery.

PARTNER WITH PROVEN INDUSTRY LEADERS

Hewlett Packard Enterprise and NVIDIA® are advancing the science of drug discovery with better insight, greater productivity, and faster time to discovery. We offer a combination of industry-leading technologies that redefine the possibilities of life sciences. Designed to manage and analyze massive amounts of data, these solutions facilitate end-to-end workflows to accelerate life-changing work and improve healthcare outcomes.

Supported by a rich independent software vendor (ISV) ecosystem, HPE and NVIDIA offer comprehensive solutions and best practices for reinventing life sciences operations. Organizations around the world are leveraging these impressive capabilities to overcome the challenges of diverse data workloads across geographies, functional teams, and multidisciplinary projects.

Our robust AI platform is built on HPE systems that are NVIDIA-certified and enable GPU-accelerated applications for supercharging the drug discovery process to help maximize ROI. The platform combines compute, storage, interconnects, software, and services for an end-to-end solution. HPE delivers these solutions on-premises, hybrid, or pay-per-use to help simplify system and data management, reduce costs and complexity, and scale to deliver excellent performance. Organizations can choose from an extensive selection of HPE systems that are engineered for AI and powered by NVIDIA GPUs to harness unparalleled processing at any scale.





In addition to vast performance gains over CPU-based platforms, GPU-based HPE systems come with NVIDIA GPUs as well as [NVIDIA software tools](#) to help optimize workflows that help with AI model development, deployment, and maintenance for accelerated workflows in drug discovery. NVIDIA Enterprise AI is an end-to-end, cloud-native suite of AI and data science tools and frameworks customized and exclusively certified by NVIDIA to run on VMware vSphere® with NVIDIA-certified systems. It includes key enabling technologies and software from NVIDIA for rapid deployment, management, and scaling of AI workloads in the modern hybrid cloud. The software delivers high sensitivity and precision for drug discovery, so you can achieve results that are [99.9% accurate](#). For GPU-powered [NVIDIA Clara Parabricks Pipelines](#) greatly outpace CPU-based workflows with similar accuracy.

NVIDIA Clara Discovery is designed to support cross-disciplinary workflows. The software brings AI to every stage of the drug discovery process by accelerating computational discovery applications with support for research in computational chemistry, genomics, proteomics, microscopy, virtual screening, visualization, and natural language processing.

NVIDIA Clara Discovery supports life sciences workflows with NVIDIA Clara Parabricks Pipelines, a core turnkey software component of the AI platform. NVIDIA Clara Parabricks Pipelines significantly accelerates genomic data analysis on-premises or in the cloud. The software employs AI for somatic and germline pipelines such as the genome analysis toolkit (GATK) and DeepVariant as well as supporting reference mapping for DNA and RNA-based applications. Event-driven insights require multiple threads of implementation at once, making them incredibly precise and time-sensitive. For many applications, the window of opportunity for insight is measured in microseconds. The decision loop must complete data capture, analysis, and implement an action immediately. If the process takes too long, the insight is no longer viable.

NVIDIA Clara Parabricks Pipelines is designed for comprehensive and high-throughput population variant calling, accelerating entire workflows. The entire pipeline is run using one compute node and does not incur any overhead of distributing data, orchestrating workflows, or reducing accuracy. The total implementation time of the GATK best practices pipeline [can be reduced dramatically to 59x](#) by using NVIDIA Clara Parabricks Pipelines software on a GPU-accelerated HPE system.

HPE and NVIDIA work closely with drug discovery ISVs to help optimize codes across genomics, computational chemistry, and structural biology for speed-of-light performance. Whether building AI for training a natural language querying tool or mapping the relationships between diseases, genes, and drugs, the software gives organizations the tools to accelerate value creation. Now, workloads that once took weeks take days, and workloads that took hours take minutes.



Solution overview

Resources

hpe.com/us/en/solutions/healthcare.html

hpe.com/us/en/solutions/hpc-high-performance-computing/nvidia-collaboration.html

nvidia.com/en-us/clara/genomics/

hpe.com/us/en/services/pointnext.html

hpe.com/us/en/greenlake.html

hpe.com/us/en/greenlake/machine-learning.html

hpe.com/us/en/greenlake/vdi.html

STREAMLINE YOUR AI DEPLOYMENT

HPE Pointnext Services offers a broad spectrum of professional, technical, and advisory support for drug discovery—from services like application tuning to more integrated advisory offerings such as project management, on-site consulting, and solution architecture consulting. HPE Pointnext Services makes it easy to transform, allowing you to focus on accelerating the performance and impact of drug discovery. Our experts collaborate with you to plan and build your ideal life sciences solutions. We determine your specific goals, application requirements, and potential roadblocks and even help you manage your technology environment after deployment.

HPE provides flexible deployment options so that life sciences research institutions, pharma, and biotech can choose how they utilize our landmark solutions.

HPE GreenLake cloud services give organizations a choice on how they utilize AI. We provide the agility, and scalability of the cloud with the security, simplicity, and control of on-premises IT. Our cloud service business and delivery model leverages data and applications across your operating environments and delivers them at any location, from edge to cloud. We offer flexible services for you to get started quickly and scale up or down as needed to handle your biggest life sciences and AI workloads. You benefit from a cloud experience when you need it, through a consumption-based model that helps you avoid heavy up-front investments and expensive overprovisioning by only paying for what you use. Now, you can easily deploy resources, manage costs, and forecast capacity—all from one intuitive platform. HPE GreenLake can manage the entire platform for you with cloud-native, zero-trust security. With fully managed cloud services, you can focus on your life sciences goals to achieve better clinical and patient outcomes.

Now, you can deploy an AI platform on-premises. Align IT economics with your AI objectives and simplify your IT operations, leveraging the unmatched speed and capacity to make faster decisions and reduce time to the next medical breakthrough.

PREPARE TO INNOVATE NOW

AI is revolutionizing drug discovery workflows. Enabling deep and immediate insights is the key to bringing lifesaving drugs and treatments to market faster.

As more organizations implement and scale solutions to facilitate research at the cutting-edge of drug discovery, they will need reliable partners with extensive AI and life sciences expertise. As market leaders in life sciences solutions, HPE and NVIDIA are disrupting the industry and powering some of the most demanding research and production environments in the world.

Together, we can help prepare every organization to deliver unprecedented health outcomes through better drugs, vaccines, therapies, and personalized healthcare. Our solutions are extremely agile and scalable to achieve the next scientific advancement, and we are committed to empowering your success.

Let us help you pioneer the future of life sciences. [Contact us](#) today.

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