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NVIDIA Announces BioNeMo Agent Toolkit

June 24, 2026 | News

The toolkit gives AI agents domain-specific tools for life sciences workflows spanning biology, chemistry, genomics and drug discovery.



NVIDIA announced NVIDIA BioNeMo Agent Toolkit, which provides domain-specific tools and skills for the agentic life sciences era.

Including more than a decade's worth of NVIDIA life sciences libraries, tools and open models, the toolkit enables AI agents, scientists and labs to work together by gathering evidence, reasoning across findings, running computational experiments and recommending the next best steps to accelerate discovery.

It gives any agent or AI platform — from general-purpose assistants to specialized scientific agents, software platforms and in-house biopharma systems — the tools needed to synthesize and summarize scientific knowledge, call models, evaluate results, reason and execute next actions.

The toolkit includes NVIDIA BioNeMo and is powered by NVIDIA NIM microservices, NVIDIA Parabricks, NVIDIA NeMo and NVIDIA Nemotron technologies, along with accelerated computing and skills — providing an open and trusted foundation for agentic life sciences.

More than 50 leading companies are already using it to advance scientific discovery, tapping into agent-callable skills for tasks including protein structure prediction, molecular docking, generative chemistry, genomic analysis, protein design and biomarker discovery.

"Frontier models are the brains. BioNeMo is the scientific toolbox. Together, they give AI agents the skills of a PhD research assistant and the speed of a supercomputer," said Jensen Huang, founder and CEO of NVIDIA. "For the first time, researchers can build AI agents that understand scientific knowledge, use scientific tools and execute scientific workflows. This is a new way to do science — one that can dramatically accelerate discovery across biology, chemistry, genomics and medicine."

Open model and research organizations — including the Arc Institute, Open Molecular Software Foundation and the University of Washington's Institute for Protein Design (IPD) — are working with NVIDIA to use BioNeMo to advance frontier models and make them more accessible through agent-ready workflows. The IPD collaboration has accelerated

runtimes for state-of-the-art biodesign models like RosettaFold3, resulting in 2 times faster performance than the prior-generation model, and many additional applications to accelerate protein design efforts are ongoing, giving researchers tools at a scale and cost not before possible.

“Every tool we’ve built for protein design is only as powerful as the scientists who can efficiently access it,” said David Baker, professor of biochemistry at the University of Washington School of Medicine and director of the Institute for Protein Design. “The next leap in science won’t come from a single discovery; it will come from the speed of iterative designs and agents that can repeatedly reason through the complexity of biology at a speed humans never could.”

Agent-Ready Tools and Skills for Life Sciences

Life sciences is one of the world’s most important scientific frontiers, with global scientific R&D reaching $3.8 trillion and annual pharmaceutical budgets approaching $300 billion.

Agentic workflows can help the industry iterate faster while reducing costs and maximizing the probability of success. With the toolkit allowing developers to transform general-purpose agents into life sciences agents in minutes, researchers can run experiments faster, continuously learn from results and close the loop between hypothesis and discovery, with some companies extending this iteration into physical labs.

A general-purpose agent can struggle to navigate scientific workflows efficiently, needing to infer the correct tools, inputs, outputs and biological meaning along the way. With BioNeMo Agent Toolkit, agents can call the right tools, interpret results more accurately and gain scientific insights faster and more reliably.

NVIDIA is optimizing the entire BioNeMo platform by turning libraries, models and frameworks into agent-callable tools.

This includes harnessing NVIDIA Agent Toolkit technologies such as NVIDIA Nemotron open models for the reasoning foundation, the NVIDIA NeMo RL library for reinforcement learning and NVIDIA NemoClaw blueprints for secure, private agents that can reason across tasks, call tools and interact with data continuously.

NVIDIA NIM microservices help agents call models and perform tasks. The NVIDIA OpenShell runtime provides a controlled executable environment.

The toolkit’s components enable agents to complete workflows such as:

- **Virtual Screening:** Agents can help researchers identify small-molecule drug candidates by generating and screening compounds, docking them to a target, predicting binding strength and filtering for drug-like properties. Then, the agent can output which candidates should be prioritized, compressing screening timelines from days to minutes.
- **Genomic Analysis and Target Discovery:** Agents can help researchers transform raw sequencing data into prioritized genetic insights and biological targets. NVIDIA Parabricks accelerates alignment and variant calling, while genomic foundation models score variant effects and the agent ranks the most disease-relevant candidates for further study.
- **Protein Binder Design:** Agents can help researchers design and validate candidates computationally before work begins, compressing traditionally labor-intensive design work.
- **Deep Biomedical Research:** Agents connect real-world data to reasoning models to improve the efficiency and accuracy of various scientific and clinical development processes, including literature review, protocol generation, clinical trial screening and pharmacovigilance with the NVIDIA Biomedical AI-Q Research Agent.
- **Medical Imaging Analysis**: Agents can help researchers process, segment, synthesize and reason over medical imaging data to support biomarker discovery, accelerating evidence generation across research workflows.

Life Sciences Ecosystem Builds With NVIDIA BioNeMo

Companies across the technology and life sciences ecosystem are using the toolkit to advance agentic workflows.

Frontier labs and scientific agent builders including Anthropic, Edison Scientific, Lila Sciences, OpenAI and Owkin are integrating with BioNeMo to help agents move from answering questions to completing scientific work. NVIDIA accelerated models and analysis libraries help shorten the time from hypothesis to insight.

Scientific data and workflow platforms from Benchling, Certara, Databricks, Snowflake and Seqera are using BioNeMo Agent Toolkit to connect data systems with AI-powered science. BioNeMo skills can help agents query biological and chemical datasets, prepare model-ready inputs, launch reproducible workflows, analyze outputs and return insights directly within the platforms scientists and data teams already use daily.

Diagnostics and pharmaceutical companies including Lilly and Natera are using BioNeMo Agent Toolkit to scale repeatable agentic workflows across discovery, translational research and clinical insight.

AI-native biology companies including Boltz, Basecamp Research, Chai Discovery, Dyno, PerturbAI and Proxima have collaborated with NVIDIA to develop tools to accelerate model-powered therapeutic design workflows.

Computer-aided drug discovery software providers including Dassault Systèmes, Cadence (OpenEye) and Schrödinger are integrating the toolkit's capabilities into scientific applications used across discovery teams. Then, agents can help orchestrate molecular generation, docking and prediction, turning computer-aided design platforms into systems where researchers can ask questions, launch analyses and identify next-best actions faster.

Lab instruments and automation companies including Automata, HighRes, Tecan, Thermo Fisher and autonomous data generation platform Medra are connecting systems with computational discovery powered by BioNeMo skills.

AI clouds and AI infrastructure companies including Baseten, Modal and Nebius are using the toolkit to help developers build life sciences workflows as reliable hosted services. By supporting BioNeMo skills and tools through scalable application programming interfaces, managed compute and production inference environments, these companies can help move agentic biology workflows from prototypes into accessible services for researchers and enterprises.