

# Achira Works With NVIDIA to Advance Molecular World Models for Agentic Discovery

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Agents are beginning to reshape how life sciences work gets done. Across biotechnology, they are becoming interfaces for complex tools, internal knowledge bases, computational models, and scientific workflows. The next step toward agentic discovery is more ambitious: moving from retrieval over known biology to design in new molecular and biological space.

That shift requires more than orchestration and search. Agents need access to evidence engines that can help scientists reason beyond known datasets, training distributions, and previously measured biology. They need systems that can generate trustworthy, physics-grounded evidence with the accessibility and latencies needed to support rapid, iterative research.

Achira is building that foundation.

## Molecular World Models for Scientific Design

Achira is building molecular world models that turn accelerated compute into a physics-grounded evidence engine through high-fidelity atomistic simulation. Rather than focusing on a narrow point solution for a single assay, target class, or workflow, we are developing foundation simulation models designed to represent and predict the behavior of molecular systems across drug targets, ligands, solvents, conformational states, and thermodynamic conditions.

The goal is not just to fit historical measurements, but to build models that can generalize where discovery teams most need help: sparse data, novel chemistry, challenging targets, novel modalities, ambiguous mechanisms, and decisions that have not yet been experimentally resolved. Achira combines first-principles quantum-derived data with experimental data to build models grounded in both molecular physics and observed biological behavior.

This reflects a broader shift in scientific AI. Instead of treating discovery as a collection of isolated prediction tasks, Achira is building a more general physical modeling layer that can be reused across a wide range of scientific questions. Just as foundation models in AI created a shared framework for many downstream tasks, molecular world models have the potential to provide a shared foundation for scientific reasoning, evidence generation, and design in chemistry and biology.

## From Known Biology to New Molecular Space

Many of the most important questions in drug discovery sit outside what has already been measured:

- Which binding mode is most plausible?
- Which compound series deserves another design cycle?
- Which modification will drive allosteric modulation of the target?
- Which molecular interaction is driving activity?
- Which candidate should be prioritized before synthesis?

These are not simply retrieval questions. They require models that can generate evidence, and [NVIDIA BioNeMo Agent Toolkit](#) is helping establish the agentic layer for life sciences through models, tools, and workflows that can help scientists move from conversation to scientific work.

The BioNeMo Agent Toolkit is NVIDIA's open platform that turns any AI agent into an autonomous life sciences scientist. It gives AI agents, software platforms and biopharma systems immediate access to NVIDIA's full life science stack. It is harness-agnostic, integrating with both the leading open models and proprietary models.

Achira's work extends that idea into new molecular space by contributing a complementary foundation: a physics-grounded evidence engine for design questions that cannot be answered by retrieval alone.



Molecular world models can give agents access to simulation-derived evidence for tasks such as hypothesis testing, molecular design, virtual screening, protein-ligand reasoning, and candidate prioritization. In practical terms, this can help scientists ask better questions, run more informed computational experiments, and allocate scarce experimental resources more effectively.

The combination is important. The [BioNeMo Agent Toolkit](#) can provide the agentic layer for life sciences, while Achira's molecular world models can contribute a physics-grounded evidence engine for scientific design. Together, these capabilities can help move life-science AI from knowledge access toward physically grounded discovery.

## **Toward a Practical Foundation for Agentic Discovery**

Agentic discovery will not be defined only by better interfaces to scientific workflows. It will be defined by whether agents can help generate credible evidence, reason across alternatives, and support better decisions in the face of uncertainty.

Achira is building one of the foundations for that future and will help move life-science AI from retrieval over known biology and discovery through experiments toward physically grounded design in new molecular space, shifting search and design from experiment to computation.

For more information and open roles please visit [achira.ai](https://achira.ai)

