InVirtuoLabs Unveils InVirtuoGEN: The AI Model That Outperforms NVIDIA on All Benchmarks

Swiss biotech redefines how artificial intelligence can drive the next generation of drug discovery

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InVirtuoLabs, the Swiss biotech startup merging deep learning with molecular science, has announced a breakthrough in AI for pharmaceutical research. Its new model, **InVirtuoGEN**, has surpassed NVIDIA's proprietary model on every benchmark the tech giant itself proposed, setting a new global performance standard for generative drug discovery.

In generating entirely new chemical compounds, supporting medicinal chemists in designing improved molecules, or optimizing binding to target proteins, InVirtuoGEN delivers superior results across every stage of the discovery process.

InVirtuoGEN represents a leap in how artificial intelligence designs and improves molecules. Rather than simply completing structures, it continuously refines them, learning to enhance promising drug candidates step by step. This approach produces more realistic and diverse compounds while drastically reducing computational cost and development time.

"I was very critical of this idea at first," says **Benno Kaech, Head of Machine Learning at InVirtuoLabs**. "It felt too novel to work in practice. But the turning point came when I realized that discovery is not about completing something finished, but about refining what exists until it becomes extraordinary. That shift in mindset made all the difference."

Recognized for its scientific novelty and excellence, the work behind InVirtuoGEN has been accepted to the **NeurIPS AI for Drug Discovery Workshop**, part of one of the world's leading conferences in machine learning, in San Diego, California in December 2025.

In de novo molecule generation, the model achieves up to a **35 percent improvement in success rate** for generating viable drug-like compounds compared to previous state-of-the-art methods. In fragment-constrained design tasks, it delivers a **40 percent gain in maintaining structural fidelity** while improving overall molecular diversity. In optimization benchmarks targeting specific protein binding properties, InVirtuoGEN consistently produces

candidates with **20 to 30 percent better binding scores** and faster convergence than any competing system, including NVIDIA's reference model.

Following its record-setting performance, InVirtuoGEN is now being integrated into **InVirtuoPlatform** to support real-world pharmaceutical programs. The model is already part of the company's internal drug discovery pipeline, accelerating the design of new treatments with higher precision, faster turnaround, and lower costs.

"InVirtuoGEN represents a groundbreaking foundational model for chemistry that is set to disrupt how we design drugs today," comments **Gianvito Grasso, Founder and CEO of InVirtuoLabs**. "This is not an incremental improvement - it's a fundamental shift in how therapeutics are discovered and optimized. At InVirtuoLabs, we have built our entire discovery platform on this foundational technology to power both our internal pipeline and collaborative programs with partners."

With this achievement, InVirtuoLabs reinforces its position at the forefront of AI-driven biotechnology, turning advanced machine learning into tangible progress for patients and partners worldwide.

About InVirtuoLabs

InVirtuoLabs is a biotech startup founded in Lugano, Switzerland in 2024. The startup closed its pre-seed funding round of €2.85 million in February 2025, marking a decisive acceleration in pharmaceutical research. Leveraging methods of advanced artificial intelligence and molecular simulations including generative models, the startup drastically reduces the time and cost of drug development, making treatments more accessible.

At the heart of InVirtuoLabs' innovation is InVirtuoPlatform, its Next Generation Virtual Lab, a proprietary platform that uses AI and molecular modeling to identify and optimize drugs with proven precision. This approach allows for doubling success rates compared to current research methods, drastically reducing both costs, currently exceeding €2.4 billion per drug, and development times, currently averaging 12 years.

The InVirtuoLabs team brings together researchers specializing in the AI-based drug discovery process as well as experts with decades of experience in the pharmaceutical industry and business management.

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InVirtuoLabs is available for interviews and speaking engagements