MIT and Recursion Release Boltz-2: Next Generation AI Model to Predict Binding Affinity at Unprecedented Speed, Scale, and Accuracy

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- Boltz-2 is the first biomolecular co-folding model to combine structure and binding affinity prediction, approaching the accuracy of physics-based free energy perturbation (FEP) calculations but at speeds up to 1000x faster in standard benchmarks
- The development of this open source model for academic and commercial use was a collaborative effort, combining MIT's deep academic expertise with Recursion's AI research and NVIDIA-accelerated supercomputer, BioHive-2

Salt Lake City, UT, June 06, 2025 (GLOBE NEWSWIRE) -- Researchers at the Massachusetts Institute of Technology (MIT) Computer Science and Artificial Intelligence Lab (CSAIL) and Jameel Clinic, alongside TechBio company Recursion (NASDAQ: RXRX), today announced the open-source release of Boltz-2, a first of its kind biomolecular foundation model. Powered by Recursion's NVIDIA supercomputer for its training and validation, this next-generation AI model achieves best-in-class accuracy in jointly modeling complex structures and binding affinities. Boltz-2 represents the next step beyond existing biomolecular structure prediction models like AlphaFold3 and its predecessor, Boltz-1.

"Accurately predicting how strongly molecules bind has been a long-standing challenge in drug discovery—one that required novel machine learning and computer science techniques to address," said Regina Barzilay, MIT School of Engineering Distinguished Professor for AI and Health, AI faculty lead at Jameel Clinic and CSAIL principal investigator. "Boltz-2 not only addresses this crucial problem but also helps scientists uncover new biological insights and ask questions they couldn't before with standard approaches that are more computationally intensive. Because Boltz-2 is open-source, including its training code, scientists can easily adapt it for specific types of molecules, making it even more powerful as a tool to accelerate discovery."

Specifically, Boltz-2 marks a new era for *in silico* screening, in standard benchmarks approaching the accuracy of physics-based free energy perturbation (FEP), an industry-standard computational method used to predict the binding affinity of molecules, at **speeds up to 1000x faster**. The decrease in cost and increase in speed and scale makes large-scale and accurate virtual screening more practical than previously possible, directly addressing a critical bottleneck in small molecule discovery.

"Selecting the right molecules early is one of the most fundamental challenges in drug discovery, with implications for whether R&D programs succeed or fail," said Najat Khan, Chief R&D Officer and Chief Commercial Officer at Recursion. "By predicting both molecular structure and binding affinity simultaneously with unprecedented speed and scale, Boltz-2 gives R&D teams a powerful tool to triage more effectively and focus resources on the most promising compounds. Collaborations like this, bridging academic innovation and industry application, play an important role in advancing the field and, ultimately, improving how we develop and deliver medicines for patients."

Below are key components and differentiators of Boltz-2 vs other methods of predicting biomolecular structures and affinities:

- **Improved Affinity Prediction**: Near-FEP accuracy on the widely adopted FEP+ benchmark while being over 1,000 times faster and less computationally expensive
- **Leading Benchmark Performance**: Superior predictive power, demonstrating outperformance over all CASP16 affinity challenge participants
- **Advanced Joint Modeling**: Uniquely models 3D complex structures while jointly predicting binding affinity and protein dynamics (e.g., B-factors)
- **Controllable & Physically Realistic**: Achieves significantly improved physical plausibility using Boltz-steering and offers enhanced user control via template, method, and contact conditioning
- **Novel & Expanded Training Data**: Trained on molecular dynamics simulations, expanded distillation data, and approximately 5 million binding affinity assay measurements

In line with MIT and Recursion's commitment to making AI tools accessible for drug developers, ***Boltz-2 will be open-sourced under an MIT license***, making the model, weights, and training pipeline available for both academic and commercial use.

Boltz-2's development was led by the Boltz team at MIT under the supervision of Professors Regina Barzilay and Tommi Jaakkola alongside a team of researchers from MIT and Recursion. For more information, visit: https://boltz.bio/boltz2.

About Recursion
Recursion (NASDAQ: RXRX) is a clinical stage TechBio company leading the space by decoding biology to radically improve lives. Enabling its mission is the Recursion OS, a platform built across diverse technologies that continuously generate one of the world's largest proprietary biological and chemical datasets. Recursion leverages sophisticated machine-learning algorithms to distill from its dataset a collection of trillions of searchable relationships across biology and chemistry unconstrained by human bias. By commanding massive experimental scale — up to millions of wet lab experiments weekly — and massive computational scale — owning and operating one of the most powerful supercomputers in the world, Recursion is uniting technology, biology and chemistry to advance the future of medicine.

Recursion is headquartered in Salt Lake City, where it is a founding member of BioHive, the Utah life sciences industry collective. Recursion also has offices in Toronto, Montréal, New York, London, Oxford area, and the San Francisco Bay area. Learn more at www.Recursion.com, or connect on X (formerly Twitter) and LinkedIn.

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