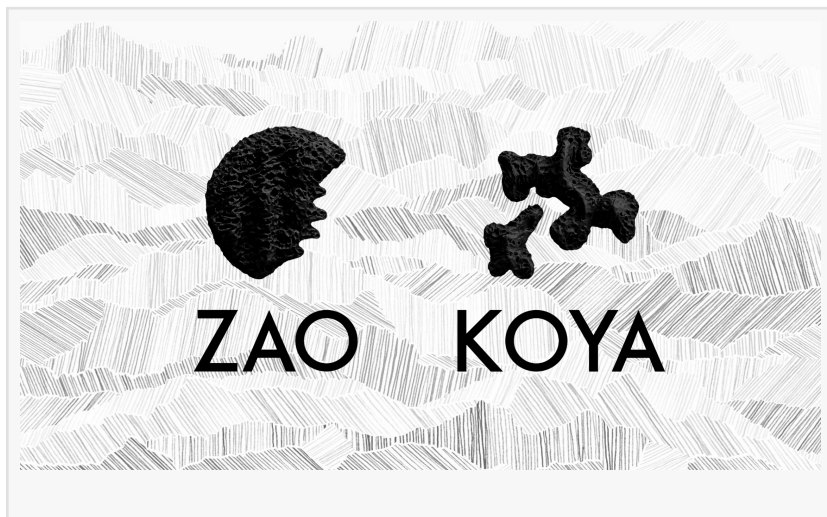


SyntheticGestalt Launches Molecular AI Models ZAO and KOYA

Available through the NVIDIA BioNeMo Agent Toolkit, advancing drug discovery where AI agents and researchers work together

MINATO CITY, TOKYO, JAPAN, July 21, 2026 /EINPresswire.com/ -- Molecular AI developer, SyntheticGestalt (headquarters: Shinjuku, Tokyo; Representative Director and CEO: Koki Shimada), today announced the launch of two molecular AI foundation models for research and development in drug discovery and chemistry: the [molecular foundation model](#) ZAO and the molecular generative model KOYA. Together, the two products use AI to support the early stages of drug discovery, from identifying promising molecules among vast numbers of candidate compounds to designing new ones, accelerating the cycle from exploration to optimization. In addition, both products can now be called from the [NVIDIA BioNeMo Agent Toolkit](#), announced by NVIDIA in June 2026, enabling their integration into AI-agent-driven drug discovery workflows.



ZAO is a molecular foundation model specialized for small-molecule information that converts the chemical structure of small molecules into data that AI can use.

Its "4D" representation, which handles the multiple 3D conformations a molecule actually adopts, captures the three-dimensional shape and flexibility that conventional methods relying on flat structures or a single conformation cannot

Pre-trained on a corpus of around 10 billion compounds, it can build high-accuracy predictive models even from as few as several hundred data points on hand

Because the output does not depend on which conformation is selected, it produces stable, reproducible features for a given molecule

Without any task-specific fine-tuning, it ranked #1 on nine public benchmark tasks including ADMET and activity prediction, achieving the world's best performance for a single general-purpose model *

KOYA is a molecular generative model that designs novel, high-affinity ligands for a target protein

while closely reflecting the intent of the medicinal chemist.

Precise design control, such as fixing a promising scaffold and growing the molecule only in the intended position and direction, directly supports lead optimization and fragment-based drug discovery

It generates new molecules while preserving the interactions to be kept with the target protein, and lets chemists specify acceptable element choices and molecular-size constraints

It automatically removes hard-to-synthesize or unrealistic structures and presents only candidates ready to move straight to evaluation, ranked with drug-likeness and ligand efficiency taken into account

Across the ten targets evaluated, it generated novel molecules that surpassed the known binding ligand in docking evaluation on eight of them

The NVIDIA BioNeMo Agent Toolkit provides capabilities such as structure prediction, molecular generation, and docking as standardized skills that AI agents can call. The company makes ZAO and KOYA available to be called from this toolkit, so that researchers can, through an agent, run the conversion of molecules into data (ZAO) and the design of novel ligands (KOYA) in the same workflow as other life-science tools.

To date, the company has demonstrated the effectiveness of its molecular AI foundation technologies in large-scale compound exploration, including a 38-billion-compound virtual screening conducted jointly with Enamine, a leading compound-library provider. It is also advancing proof-of-concept work with major domestic pharmaceutical and chemical companies. ZAO and KOYA bring to market the foundation technologies cultivated through this track record.

Koki Shimada, Representative Director and CEO of SyntheticGestalt, commented: "An era in which AI agents advance research on their own is beginning. By making ZAO and KOYA usable from the NVIDIA BioNeMo Agent Toolkit, agents can take on everything from evaluating molecules to designing them, and work together with researchers to accelerate discovery. This is the new form of drug discovery we aim to realize."

ZAO and KOYA are both offered for enterprise use. Terms of use and pricing are arranged individually for each product.

About SyntheticGestalt

SyntheticGestalt is a Tokyo-based molecular AI company. It develops and deploys molecular AI across the pharmaceutical, chemical, materials, agrochemical, cosmetics, and food industries, and since its founding in 2018 has pursued its mission of building systems that mass-produce inventions through AI. Its research projects have discovered pharmaceutical lead compounds and materials with lower environmental impact, while reducing the cost and time of exploration by up to 90% compared with conventional methods. For more information, visit

<https://www.syntheticgestalt.com>.

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