AI AT SCALE MEETS SCIENTIFIC RIGOR

NVIDIA MolMIM Integration into BIOVIA Small Molecule Therapeutics Design

Generative AI is expanding chemical space and accelerating the discovery of novel molecules. But identifying viable drug candidates requires more than rapid generation; it demands scientific validation and molecular understanding.

By integrating NVIDIA MolMIM NIM into BIOVIA Small Molecule Therapeutics Design, researchers can combine generative AI and rule-based chemical transformation for molecule generation and retrosynthetic scoring and 3D physics-based modeling for lead optimization. This combinatorial approach helps identify high-quality candidates that balance novelty, synthesizability, drug-like properties, and biological relevance while optimizing against complex Target Product Profiles (TPPs).

BIOVIA SMALL MOLECULE THERAPEUTICS DESIGN

BIOVIA offers a complete suite of solutions for small molecule therapeutics design on the **3DEXPERIENCE®** platform. These solutions are seamlessly integrated supporting scientists end-to-end, from virtual ideation to lab synthesis and testing.

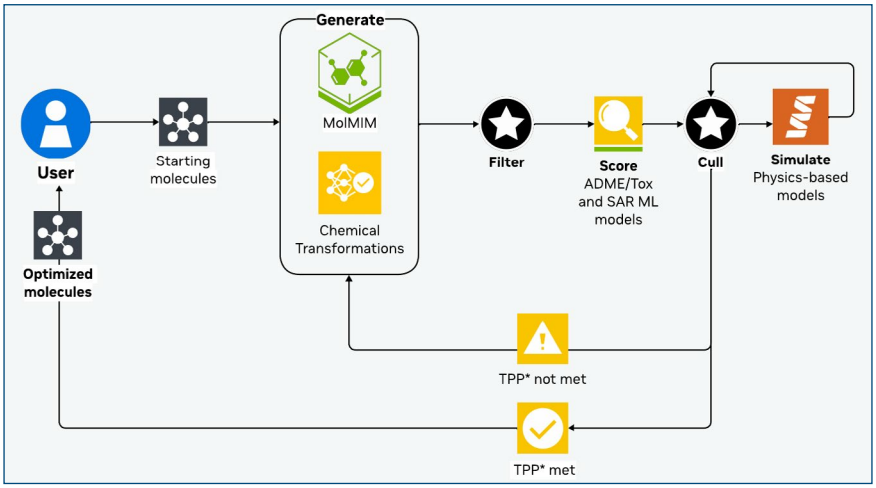
Small molecule leads are generated and optimized through:

- **Chemistry-based methods:** Uses mechanistically correct chemical transformations to generate valid structures.
- **Rule-based validation:** Ensures all generated synthesizable molecules adhere to the strict rules of organic chemistry.
- **Retrosynthesis scoring:** Prioritizes compounds based on synthetic feasibility, ensuring generated structures can be efficiently produced in the laboratory.
- **Multiparameter optimization (MPO):** Evaluates candidates against TPPs and ensure they meet exact design objectives using Machine Learning.
- **Active learning:** Connects virtual and experimental workflows to optimize leads through iterative design cycles, accelerating the design-make-test-analyze process.

THE ROLE OF NVIDIA MOLMIM

NVIDIA MolMIM is a transformer-based generative AI model designed for small molecule generation, optimization and embedding. Available as an NVIDIA Inference Microservice (NIM) within the NVIDIA BioNeMo platform, MolMIM brings advanced deep learning to molecular design.

MolMIM works by translating molecules into a "latent space," a compressed numerical representation of chemical features. This allows the model to intelligently navigate vast regions of chemical space, make controlled changes to existing molecules and generate novel structures. It then ranks these new candidates against external criteria to find the most promising options.



Integrated workflow with NVIDIA MolMIM NIM in BIOVIA Small Molecule Therapeutics Design. * TPP: Target Product Profile.

BETTER TOGETHER: GREATER THAN THE SUM OF ITS PARTS

Combining NVIDIA MolMIM with BIOVIA's chemical transformation offers a complementary approach to lead generation, where AI-driven design works together with rule-based scientific methods to identify higher-quality candidates than those with either approach alone.

The benefits include:

- **Seamless workflow alignment:** MolMIM enhances generative discovery workflows and supports iterative lead optimization and structure refinement.
- **Complementary design approaches:** MolMIM and BIOVIA chemical transformations work together to proposed chemically reasonable variations and new scaffolds.
- **Enhanced optimization:** Together with MolMIM's generative power BIOVIA's drug discovery solutions deliver superior results for Target Product Profile (TPP) optimization.
- **Expert-driven validation:** Scientists use physics-based modeling and domain expertise to identify designs with the highest experimental success potential.

KEY BENEFITS FOR THE DISCOVERY TEAMS

For discovery teams and research organizations, the integration of NVIDIA MolMIM NIM directly BIOVIA into small molecule therapeutics design improves experimental success rates and operational efficiency through:

Scalable cloud deployment

Leverage NVIDIA GPU-optimized AI microservices to support flexible, high-performance deployment across research environments.

Flexible support for teams of any size

Enable both small research teams and large pharmaceutical organizations to scale AI-driven discovery through SaaS-based workflows powered by NVIDIA technologies.

Unified platform for Scientific R&D

Connect virtual molecular design with experimental and laboratory data in a single environment, enabling drug discovery driven by Scientific AI.

Faster lead optimization

Rapidly isolate high-potential leads while filtering out unviable options early in the discovery process.

Improved candidate quality

Combine the creativity of AI with rigorous scientific methods to design more promising molecules.

Reduced research costs and shorter development timelines

Prioritize compounds with a higher likelihood of success before synthesis, saving resources and time.

By combining the scale of NVIDIA generative AI with BIOVIA's rigorous scientific validation, chemists can evaluate millions of possibilities with the precision required to choose the most viable path forward.

LEARN MORE

DASSAULT SYSTEMES