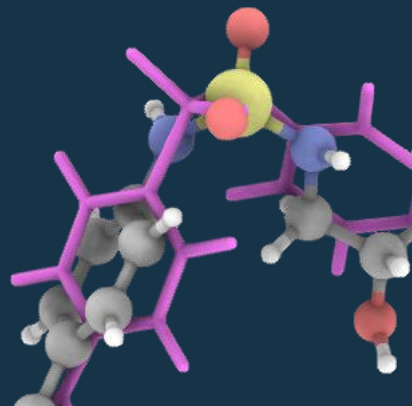
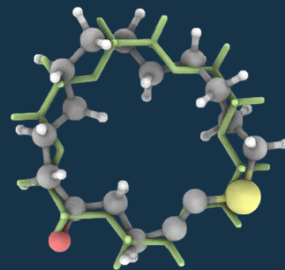
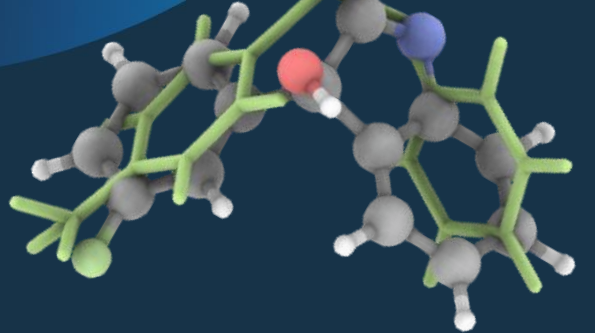




MLConfGen:

Transforming Hit Discovery
with Generative AI

Denis Sapegin / Alex Proutski | BioTechX 2026



Screening Millions to Find a Few



Traditional Virtual Screening

- Millions to billions of compounds must be enumerated and screened.
- Large-scale docking campaigns consume significant CPU/GPU resources and weeks of compute time.
- Most generated compounds are discarded before experimental evaluation.
- Cost per computational hit is driven by:

Library enumeration

Conformer generation

Docking

ADMET and solubility filtering

Iterative design cycles

Business Impact

Longer project timelines

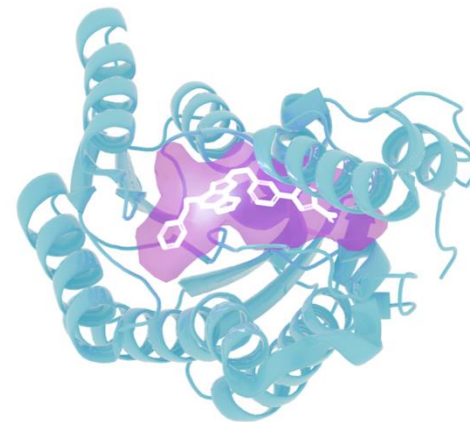
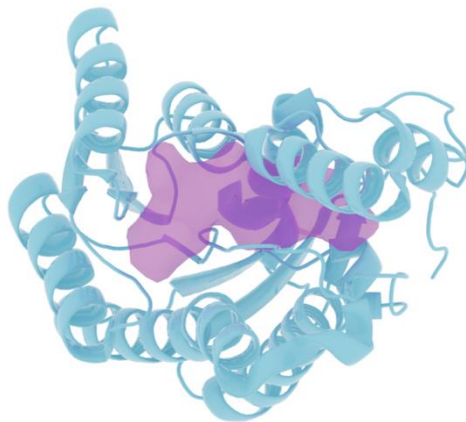
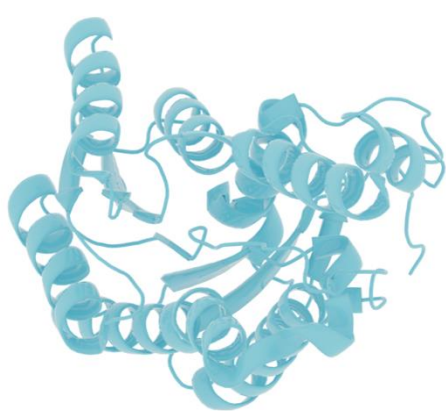
Higher infrastructure costs

Fewer design iterations per program

Delayed progression from target to hit

Result: Teams spend substantial compute and scientist time searching chemical space rather than designing promising molecules.

ML Conformer Generator – A Smarter Way to Generate Molecules



1 Identify the pocket, capture inlay geometry

< 1 sec

2 Generate ready-to-dock ligand poses

< 20 sec (50 samples)

MLConfGen: Generate Hits Instead of Screening for Them



Shift from "Enumerate & Screen" to "Generate & Optimize"

MLConfGen directly generates molecules within the desired chemical space while conditioning on:

- A reference ligand pose or Protein pocket geometry
- Desired reaction or scaffold constraints
- Custom multi-objective scoring functions

ROI Drivers

- ✓ Dramatically reduces the number of compounds requiring docking and rescoring
- ✓ Eliminates large-scale reaction enumeration workflows
- ✓ Accelerates hit generation from weeks to hours
- ✓ Reduces compute consumption per computational hit
- ✓ Enables more design-test-learn cycles within the same budget

Outcome: Lower cost per computational hit and faster lead discovery. In practice 0.4-4\$ for high-confidence comp hit *

Traditional VS:

Screen millions to find tens of hits

MLConfGen:

Generate tens of likely hits directly

Result:

10–100× fewer compounds evaluated, significantly lower compute spend, and faster time-to-hit.



Faster Discovery with Lean AI Infrastructure



MLConfGen is designed for efficient inference:

Lower GPU requirements

Faster generation
throughput

Reduced operational costs

Easier deployment across
discovery teams



Ready to be deployed on AWS,
GCP (with a click of a button),
Nebius or on-prem

Workflow

Business Value

Reaction / scaffold-conditioned generation	>	Explore relevant chemical space efficiently
Fragment growth	>	Rapid hit expansion
Linker design	>	Accelerate fragment linking campaigns
Pocket-driven generation	>	Direct structure-based design
Objective optimization	>	Generate compounds optimized for docking, solubility, and project-specific metrics
Automated hit-generation pipelines	>	Reduce manual screening effort
AI-assisted 3D medicinal chemistry	>	Enable chemists to explore ideas at the speed of thought

Add Spatially-Aware Molecular Design to Your Platform



Most AI drug discovery platforms combine existing models, workflows, and infrastructure.

Instead of building and maintaining a specialized 3D molecular generation model, integrate **MLConfGen** as a ready-to-deploy capability.

What Your Customers Get

- Pocket-conditioned molecule generation
- Pose-conditioned design
- Fragment growth and linker design
- Multi-objective optimization
- Custom fine-tuning and scoring functions

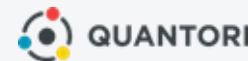
Why It Matters

- ✓ Expand platform capabilities quickly
- ✓ Differentiate your offering
- ✓ Reduce development and maintenance costs
- ✓ Deliver more value to medicinal chemists

Focus on your platform and users. We provide the spatially-aware molecular generation engine.

We are able to customise it and integrate with your models.

ML Conformer Generator: General Use Case



Integrates seamlessly with your cheminformatics workflows to enable **rapid, pocket-driven molecule design** and accelerate scaffold discovery.

Up to 10× Increase in High-Confidence Hit Rate

Objective-Guided Generation compatible with **REINVENT4** scoring

Fix Target Pharmacophore Positions During Generation

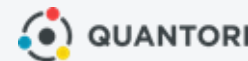
Faster molecule generation tailored to specific binding sites and 3D shapes

Generate Ligands in a ROCS-like shape-similarity manner

Generate compounds with **low-strain geometries**

Guide molecular generation using **Fragment Libraries** to ensure **synthetic accessibility**

ML Conformer Generator: Return of Investment



Generate synthesizable and shape-similar molecules faster than you search for them!

The screenshot shows the "ML Conformer Generator" web interface. At the top, a progress bar has four steps: 1. Input (checked), 2. Pocket (active), 3. Ligands, and 4. Results. The "Define Pocket" section on the left includes buttons for "Select Residues" and "Select Ligand", a text box for "Enter PDB File", and a "Generate Pocket Shape" button. Below this, it says "Pocket is created" and has a "Download STL" button. The central 3D viewer shows a protein structure with a blue mesh representing the binding pocket and red dots indicating selected residues. The "Scene" panel on the right lists "STRUCTURES" (1uyd, protein, HEAT SHOCK PROTEIN HSP 90-ALPHA) and "POCKET SHAPE" (Pocket shape).

ML Conformer Generator
Molecule Designer

1 Input
Enter PDB File

2 Pocket
Define pocket

3 Ligands
Generate candidates

4 Results
View result

Define Pocket

Select Residues Select Ligand

Select protein residues in 3D viewer (Left click) to define your binding pocket.
It is possible to select a ligand and press "Select surroundings" button to select all residues around the ligand.

CURRENT SELECTION
(A: 22, 48, 51-52, 55, 93, 96-98, 102-103, 107-108, 110-111, 135-136, 138-139, 150, 152, 162, 183-184, 186)

Generate Pocket Shape

Pocket is created Download STL

Next Step

Residue Nothing Selected Select Surroundings

Scene

STRUCTURES

- 1uyd
- protein
- HEAT SHOCK PROTEIN HSP 90-ALPHA
- ligand
- water

POCKET SHAPE

Pocket shape

Shape-aware generation: **more hits,**
fewer molecules screened.

Provide users with capabilities for live ML-
assisted molecule design

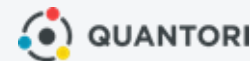
Generate Datasets and expand compound
libraries in a matter of minutes

Integrate into existing tools smoothly
through a versatile and robust API

Run Agentic workflows through MCP
Integration

Low GPU-compute cost

Molecule Designer



ML Conformer Generator
Molecule Designer

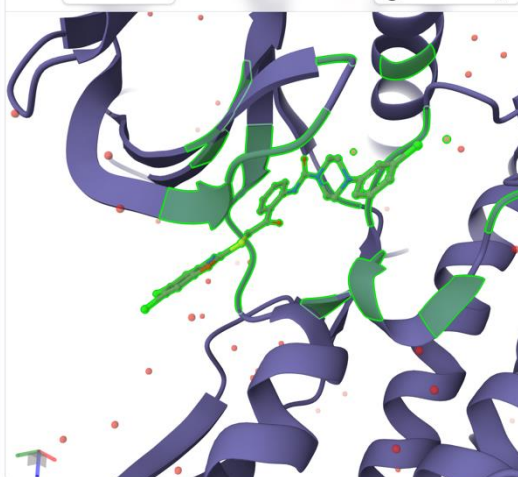
Progress: 1. Input (Enter PDB File) | 2. Pocket (Define pocket) | 3. Ligands (Generate candidates) | 4. Results (View result)

Generated Molecules [Download results](#)

View the generated ligands in the pocket.

- GEN_001 Score: 0.6 [✓ Shown in 3D Viewer](#)
- GEN_002 Score: 0.6
- GEN_003 Score: 0.5
- GEN_004 Score: 0.5

Select: Residue 42 Residues Selected [Select Surroundings](#)



Scene

STRUCTURES

- 6q8k
- protein
- Dual specificity protein kinase CLK1
- ligand
- 1, 2-ETHANEDIOL
- ~(N)2-(3-morpholin-4-ylpropyl)pyrido...
- water
- GEN_001

POCKET SHAPE

No items

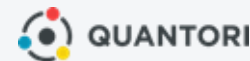
AI-assisted molecular design in the web-based 3D molecule editor

Reference-, pocket-, or fragment-driven design control

Go from design to docking in one step with ready-to-dock poses

Design at the speed of thought with real-time molecule generation

Admin UI



 ML Conformer Generator
made by Quantori

Dashboard

Tasks

Docs

Molecule Designer

Need support with getting started or going further?

We can help you with:

- User Training
- Advanced Configuration & Integration
- Custom UI Development
- Model Fine-tuning & ML Pipeline Design

Get our services designed to integrate and scale your molecular generation workflows

Available on AWS, GCP & More — Contact us to learn how we can support your team.

Help & Support

Contact Us

About

Tasks

Current Completed

Filters (10) Cancel + New task

☐ Task ID	Date	Time	Token name	Status	
☐ A9901093	06/11/25	09:00 AM	BioTech Innovations	Completed	
☒ A9901093	06/12/25	01:15 PM	GreenTech Solutions	Queued	
☒ A9901093	06/13/25	11:45 AM	Quantum Computing Corp	Queued	
☐ A9901093	06/14/25	01:15 PM	AeroDynamics Inc	Running	
☐ A9901093	06/15/25	02:30 PM	Urban Farming Co	Completed	
☐ A9901093	06/16/25	03:00 PM	NextGen Robotics	Completed	
☐ A9901093	06/17/25	04:15 PM	SmartWear Technologies	Failed	
☐ A9901093	06/18/25	05:30 PM	EcoEnergy Systems	Completed	
☐ A9901093	06/19/25	06:00 PM	HealthSync Technologies	Completed	
☐ A9901093	06/20/25	07:15 PM	FutureVision Media	Failed	
☐ A9901093	06/21/25	08:30 PM	DataWise Analytics	Queued	
☐ A9901093	06/22/25	09:45 PM	CloudSphere Networks	Running	
☐ A9901093	06/23/25	10:15 PM	Culinary Arts Labs	Queued	
☐ A9901093	06/24/25	11:30 PM	Insightful Designs	Canceled	
☐ A9901093	06/25/25	12:00 AM	SecureHome Innovations	Completed	
☐ A9901093	06/25/25	12:30 AM	Insightful Designs	Completed	

← 1 2 3 4 ... 25 26 27 →

Selected: 2 of 21 831

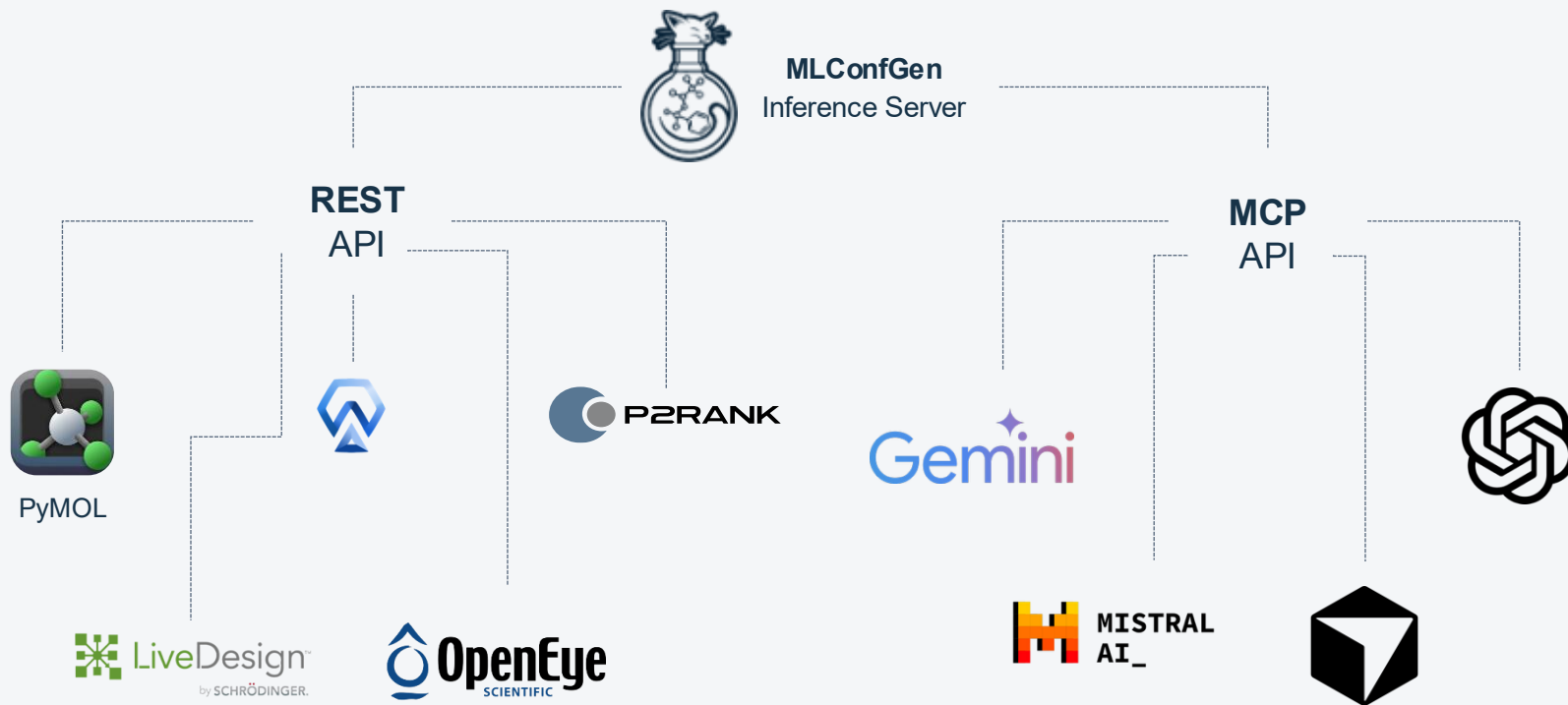
Streamlined Task Management
& Access Control

Comprehensive API
Documentation

Flexible Server Configuration

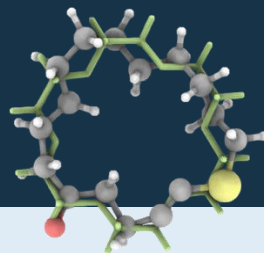
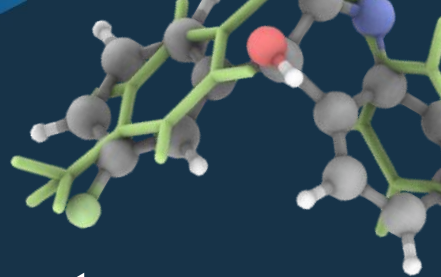
Real-Time Hardware Utilization
Dashboard

ML Conformer Generator: Integration





Bring ML Conformer Generator Into Your Pipeline



Inference as a Service

Access ready-to-use molecule generation through cloud platforms — no setup required.



Google Cloud

Open-Source Access

Use our PyPI package with pretrained weights to evaluate and experiment freely.

GitHub

Custom Training & Fine-Tuning

Adapt the model to your own chemistry, fine-tuned on your proprietary data for maximum relevance and performance.

Custom Dataset Generation

Need specialized conformers for a specific scaffold class or shape constraint? We generate high-quality training or inference datasets to match your needs.



Thank You for Attention!

Come say hi at **Booth #190**

