



Large Language Model for Drug Discovery and Medical Imaging Generative AI

Warren Tseng, Solution Architect, April 2023.



- Large Language Model (LLM) and Biology?
- Use Cases: LLM for Drug Discovery Acceleration
- NVIDIA BioNeMo
- MONAI Generative AI

Large Language Model (LLM) and Biology?



2023 Large Language Model (LLM)

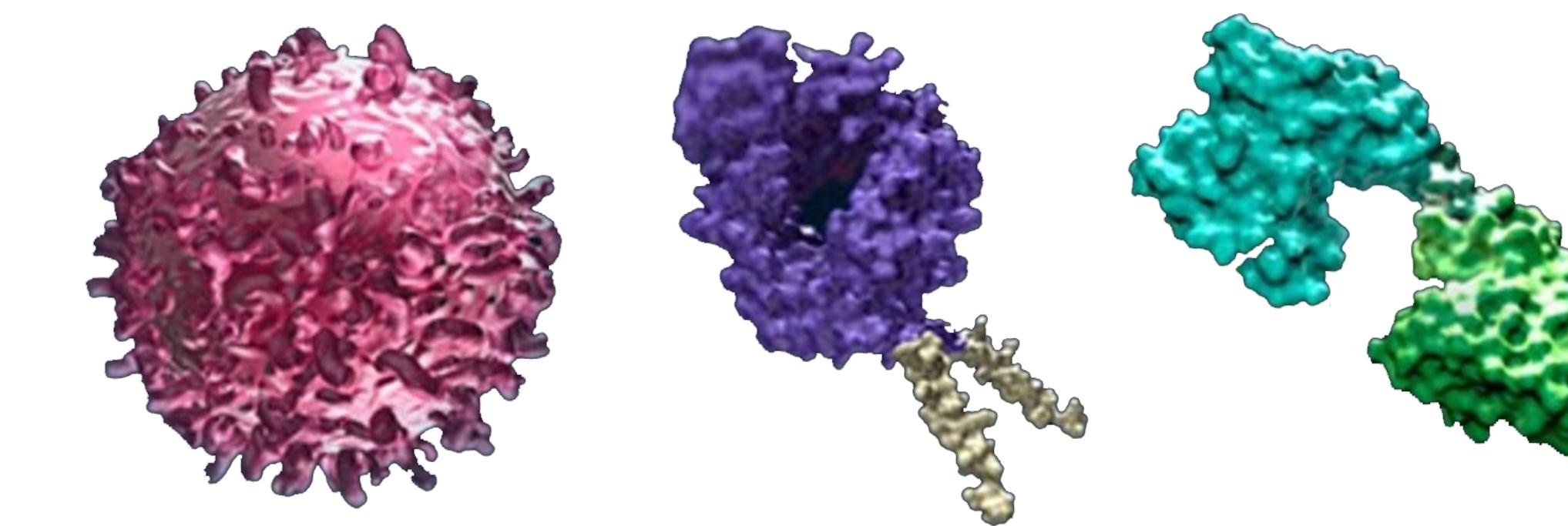
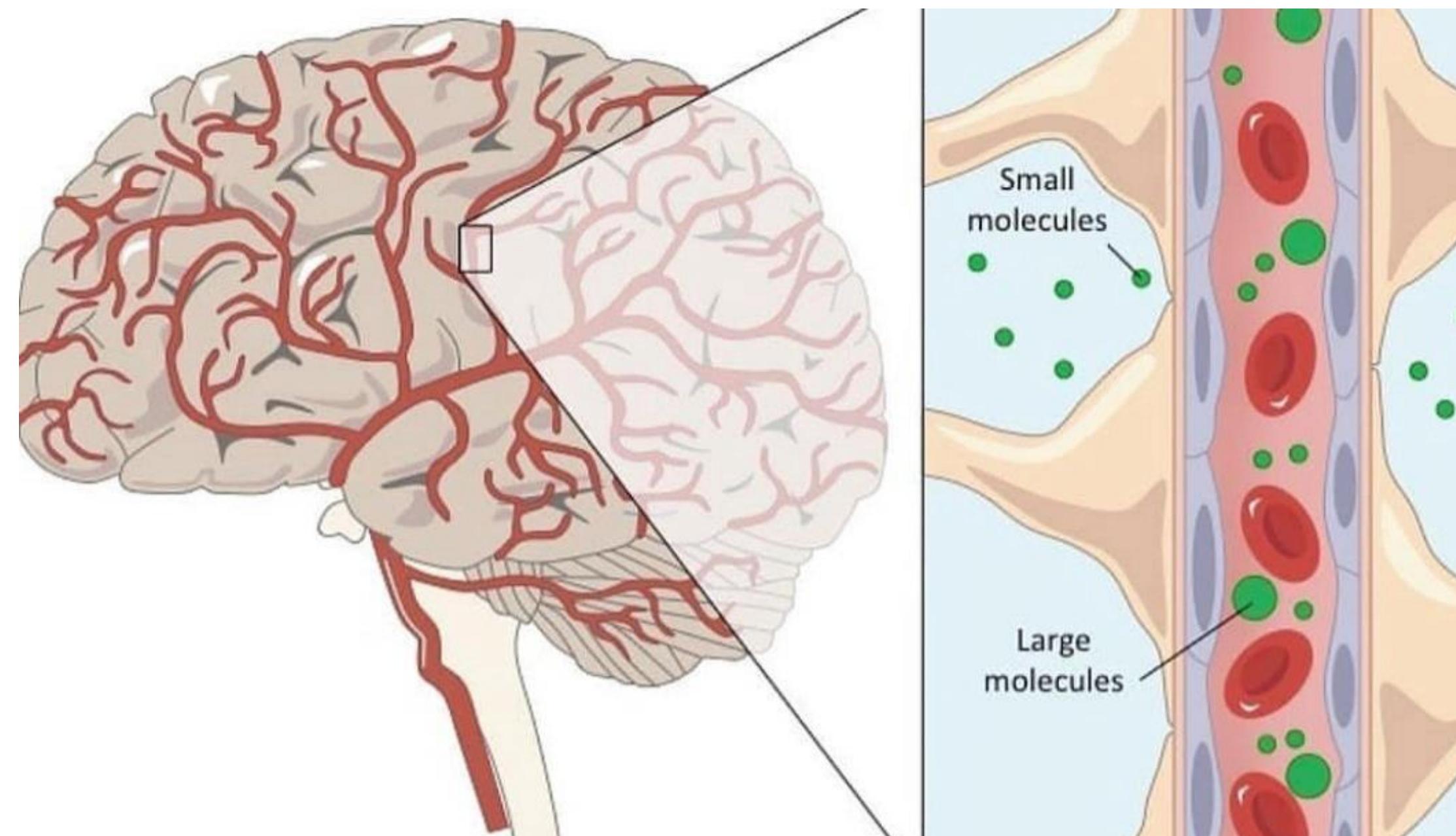
OpenAI ChatGPT
a BigScience initiative
BLOOM
176B params · 59 languages · Open-access

NEXT Forum
多模態基礎模型
Multi-Modal Foundation Model

大型語言模型 LLM
AI 2.0 線上技術論壇
AIHPC x Large Language Model
BLOOM 176B
大語言模型成果展示
Fri. 2/10 15:00-16:00
立即報名

ChatGPT/ Bloom
(SINICA, HHRI, MTK)
LLM/ Foundation Models Forums
(NTU, SINICA, NYCU, NTHU, HHRI, TWS)

ChatGPT is the “iPhone moment” for LLM/Generative AI”



Blood Brain Barrier with MegaMolBART
(CMUH, NCHC/TWS , NVAITC Joint Lab)

Anti-body – Dr Liu
(NHRI, NTU, NVAITC Joint Lab)

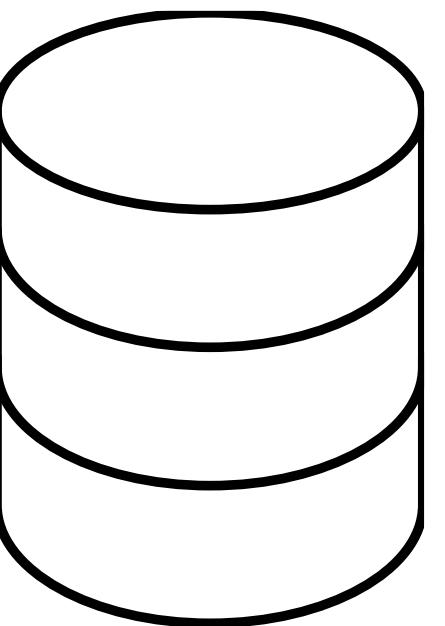
Gartner industry analyst predicts 30%+ of new drugs in 2025 will be created by LLM

Reference:

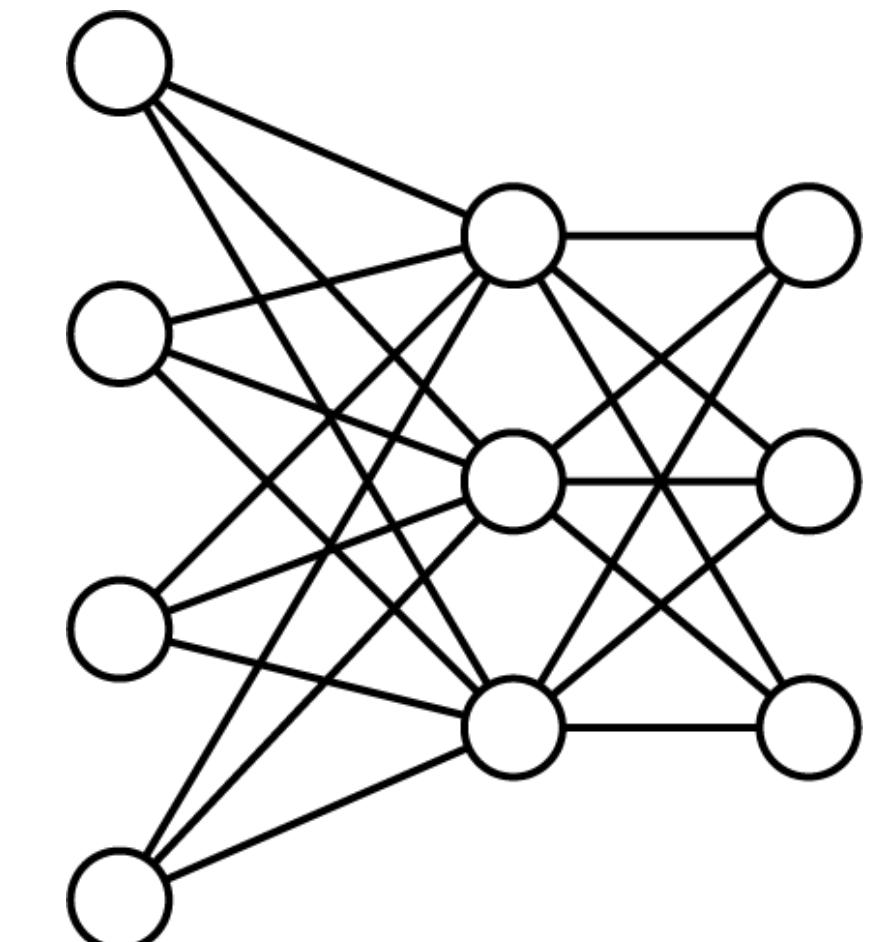
1. iPhone moment:
<https://fortune.com/2023/03/01/artificial-intelligence-ai-chatgpt-iphone-moment-bank-of-america/>
2. Gartner industry analyst:
<https://www.gartner.com/en/articles/beyond-chatgpt-the-future-of-generative-ai-for-enterprises>
3. 大語言模型線上技術論壇:
<https://tws.twcc.ai/2023/01/18/llm/>

What is Large Language Model?

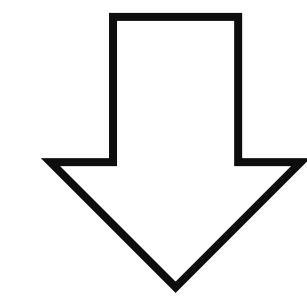
- **ChatGPT said:** “A large language model (LLM) is a language model that consists of a neural network with many parameters (usually **billions of weights** or more), and is trained on **large amounts of unlabeled text** using self-supervised learning. **LLMs can recognize, summarize, translate, predict and generate text and other content.**”



Large amounts of text data or sequence data



Billions of weights
GPT-3: 175 B
BLOOM: 176 B



Content Generation	Summarization	Translation	Chatbots	Virtual Avatars
An illustration of a small blue and silver robot sitting on a stool and painting on a canvas with a paintbrush.	A classical painting of a person in a blue robe sitting at a desk, looking down at a book or manuscript.	A close-up photograph of a person's hand holding a pen and writing on a piece of paper.	A photograph of a person's hand holding a smartphone with a "LIVE CHAT" screen showing a message exchange.	A photograph of a man in a grey shirt and glasses standing next to a white humanoid robot, both looking at a tablet device.

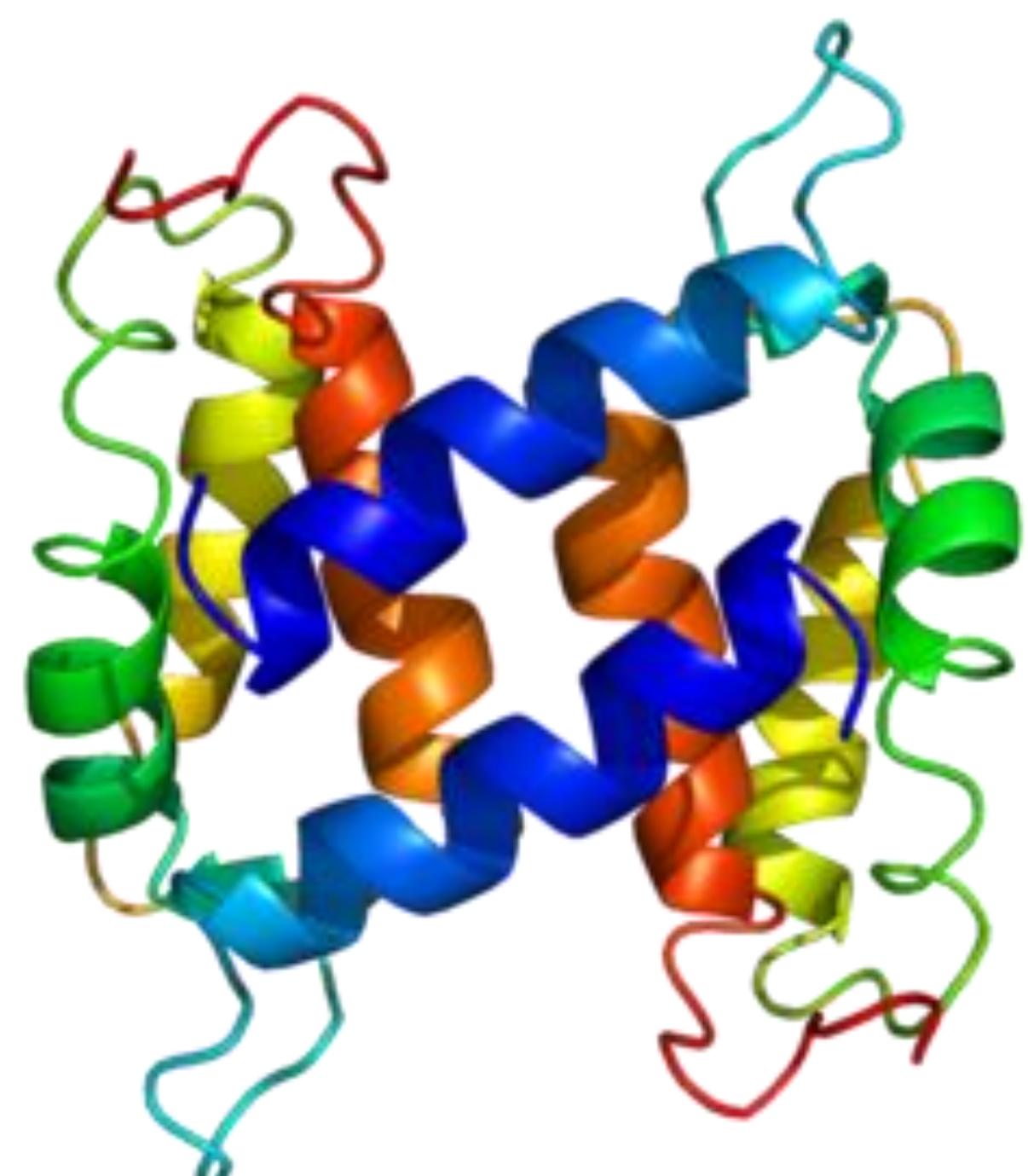
Relationship between Biology & LANGUAGE MODELS

Natural Language

Drug development is a cross-disciplinary endeavor

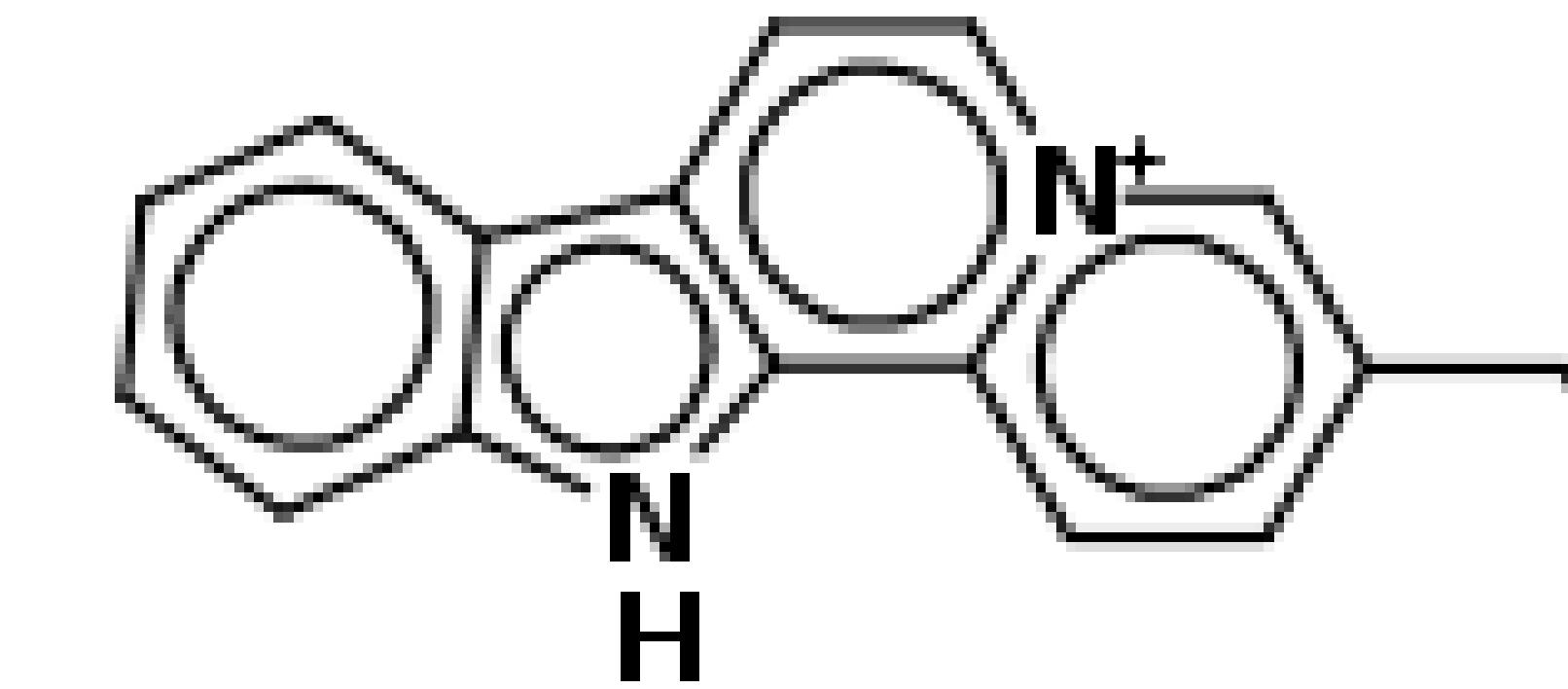
<https://catalog.ngc.nvidia.com/orgs/nvidia/collections/claradiscovery>

Language-like Series



```
ATIKVTKANTLFKIAAY  
PMMVAKKRIILRAMKRI  
ILRIKVTKANTLFKIIL  
RIKVNTLFKIILRIKV  
TNTMVAKKRITNKLISL  
ALALIRMKTLILRIKV  
KAVTKANTLFKIILRIKV  
VGGKANTLFKIILRIKV
```

FASTA Sequence

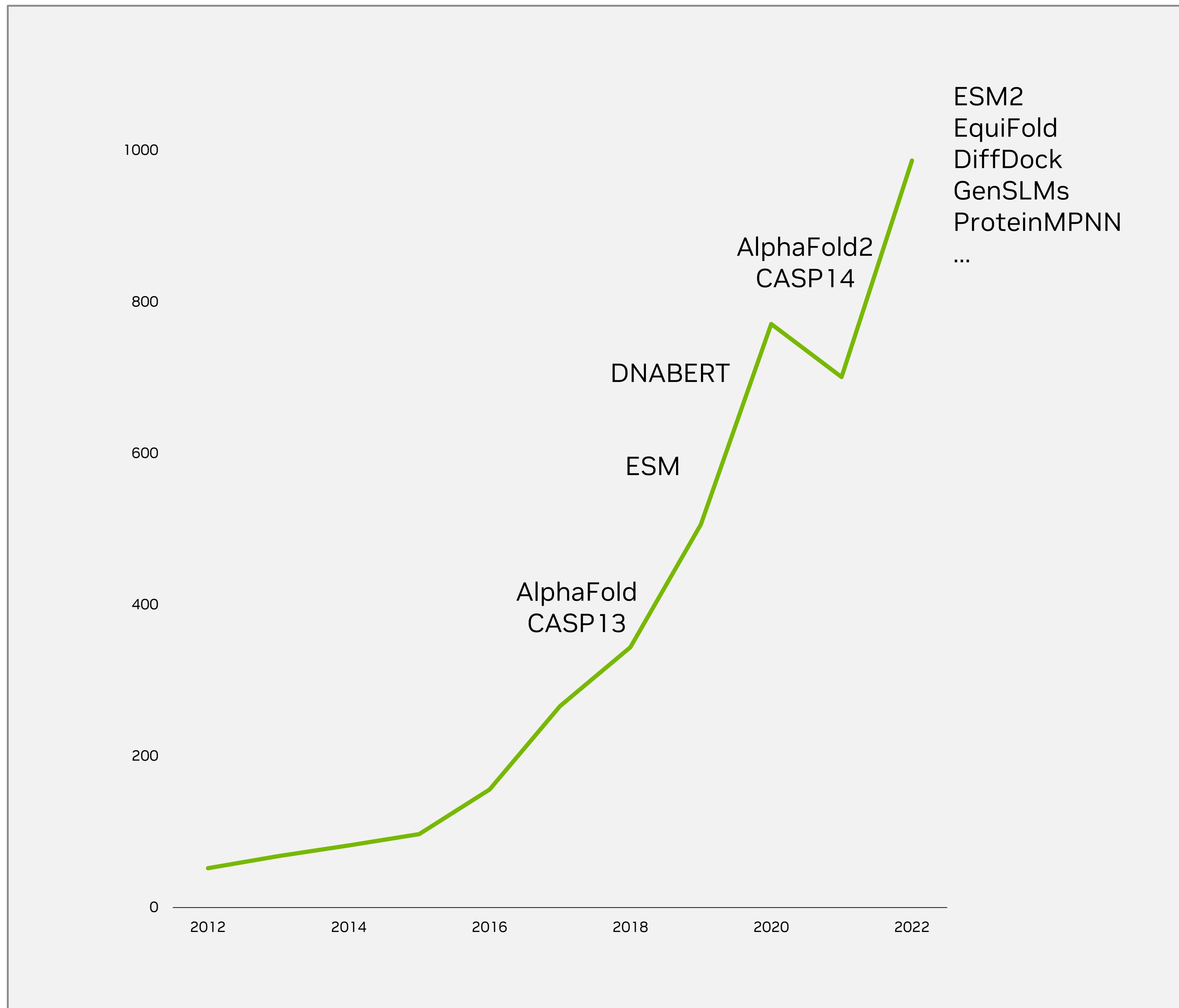


```
CCc(c1)ccc2[n+]1ccc3c2[nH]c4c3cccc4  
CCc1c[n+]2ccc3c4cccc4[nH]c3c2cc1
```

SMILES

Generative AI is Exploding in Drug Discovery

AI Published Papers

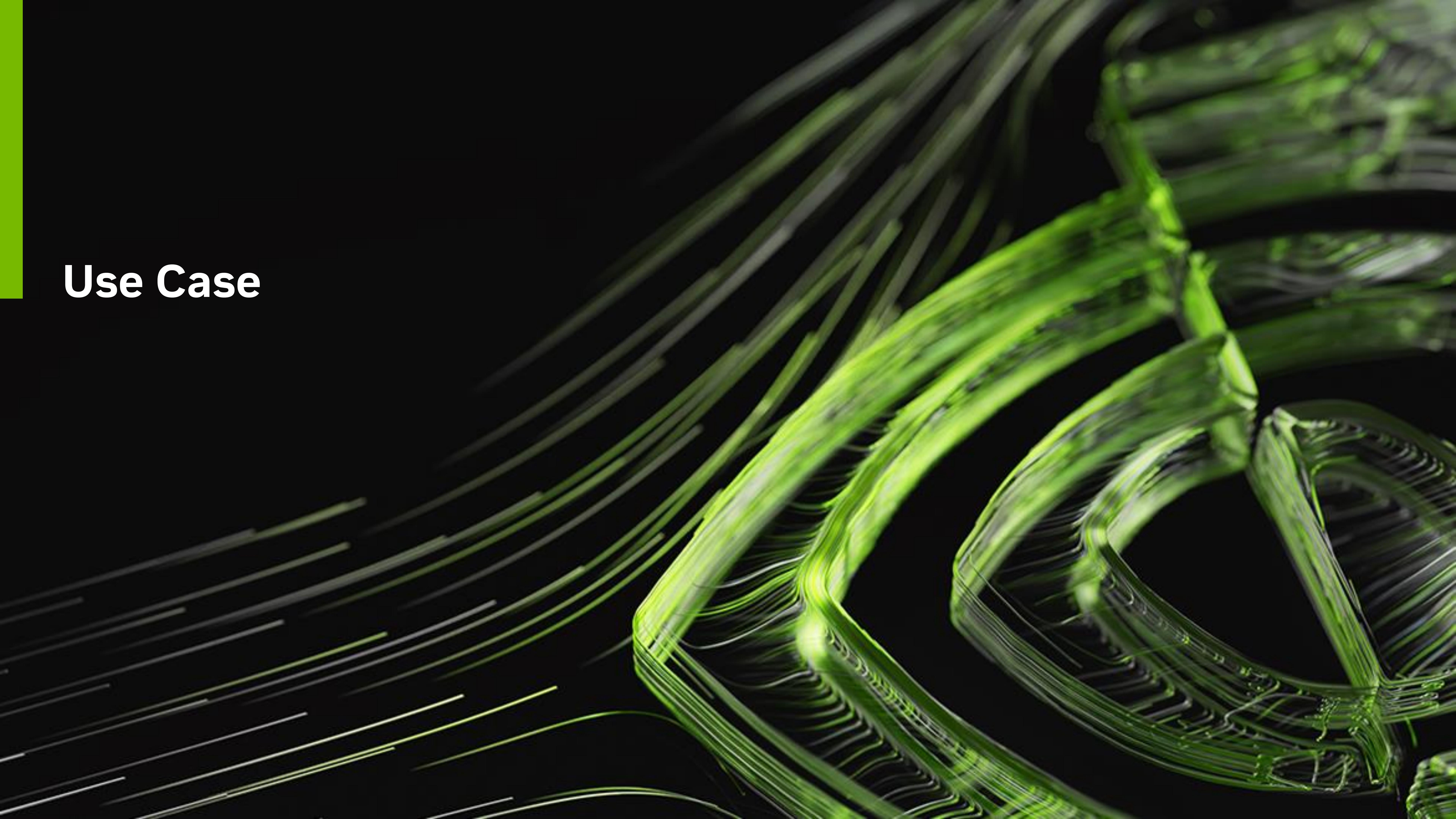


NVIDIA Joint Research

Six panels illustrating NVIDIA joint research projects in drug discovery:

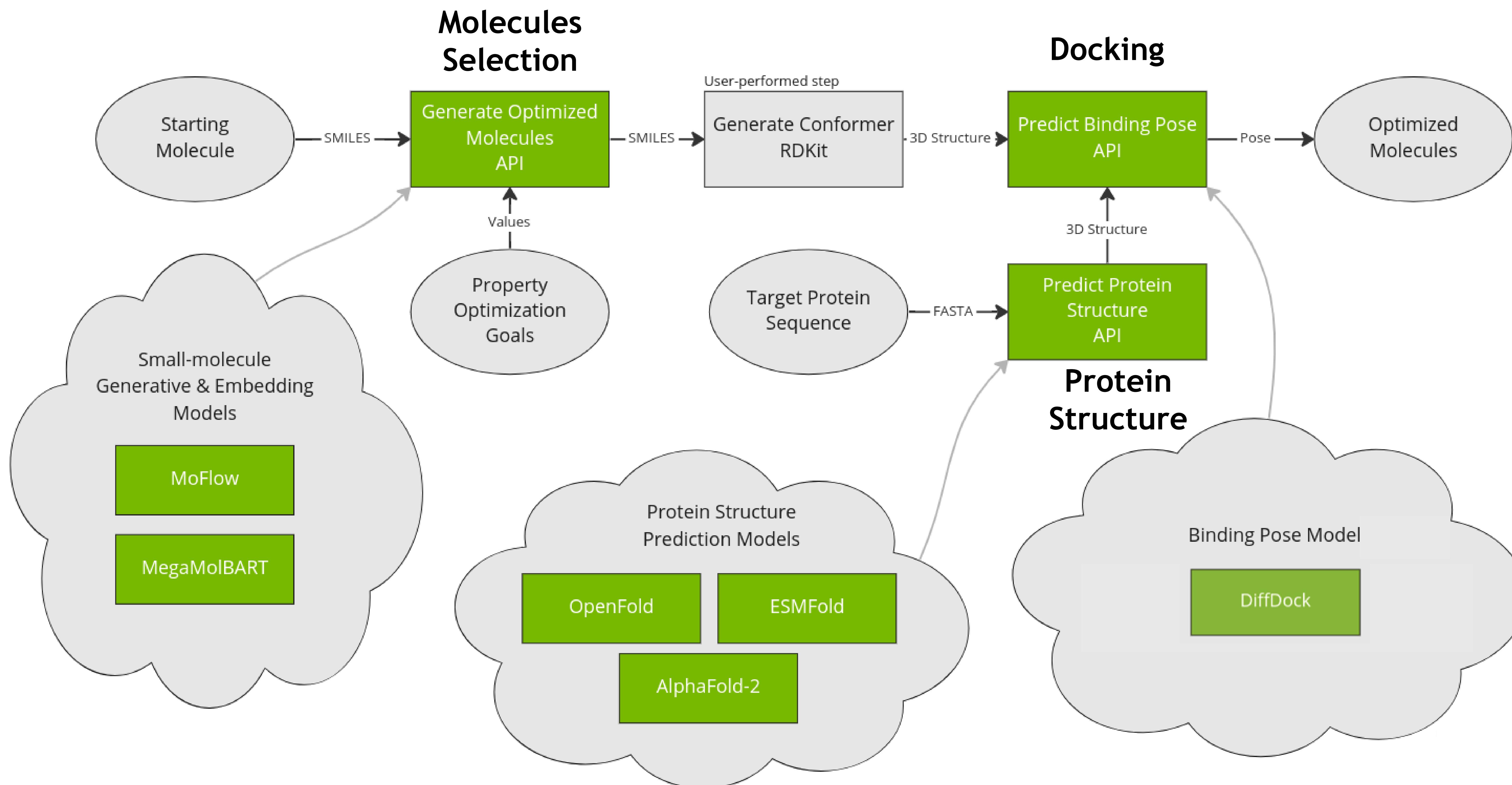
- GensLMS**: Genome-scale language models reveal SARS-CoV-2 Evolutionary Dynamics. Shows a 3D point cloud visualization.
- Nucleotide Transformer**: Building and Evaluating Robust Foundation Models for Human Genomics. Shows a DNA helix with various genomic annotations.
- MolMIM**: Improving Small Molecule Generation using Mutual Information Machine. Shows a diagram of the model architecture and a 3D molecular structure.
- ProT-VAE**: Protein Transformer Variational AutoEncoder for Functional Protein Design. Shows a 3D protein-ligand complex.
- NeuralPlexer**: Dynamic-Backbone Protein-Ligand Structure Prediction with Multiscale Generative Diffusion Models. Shows a 3D protein-ligand complex.
- MegaMoBART**: Generally Applicable Chemical AI Models with Large-Scale Pretrained Transformers. Shows a grid of chemical structures.

Use Case



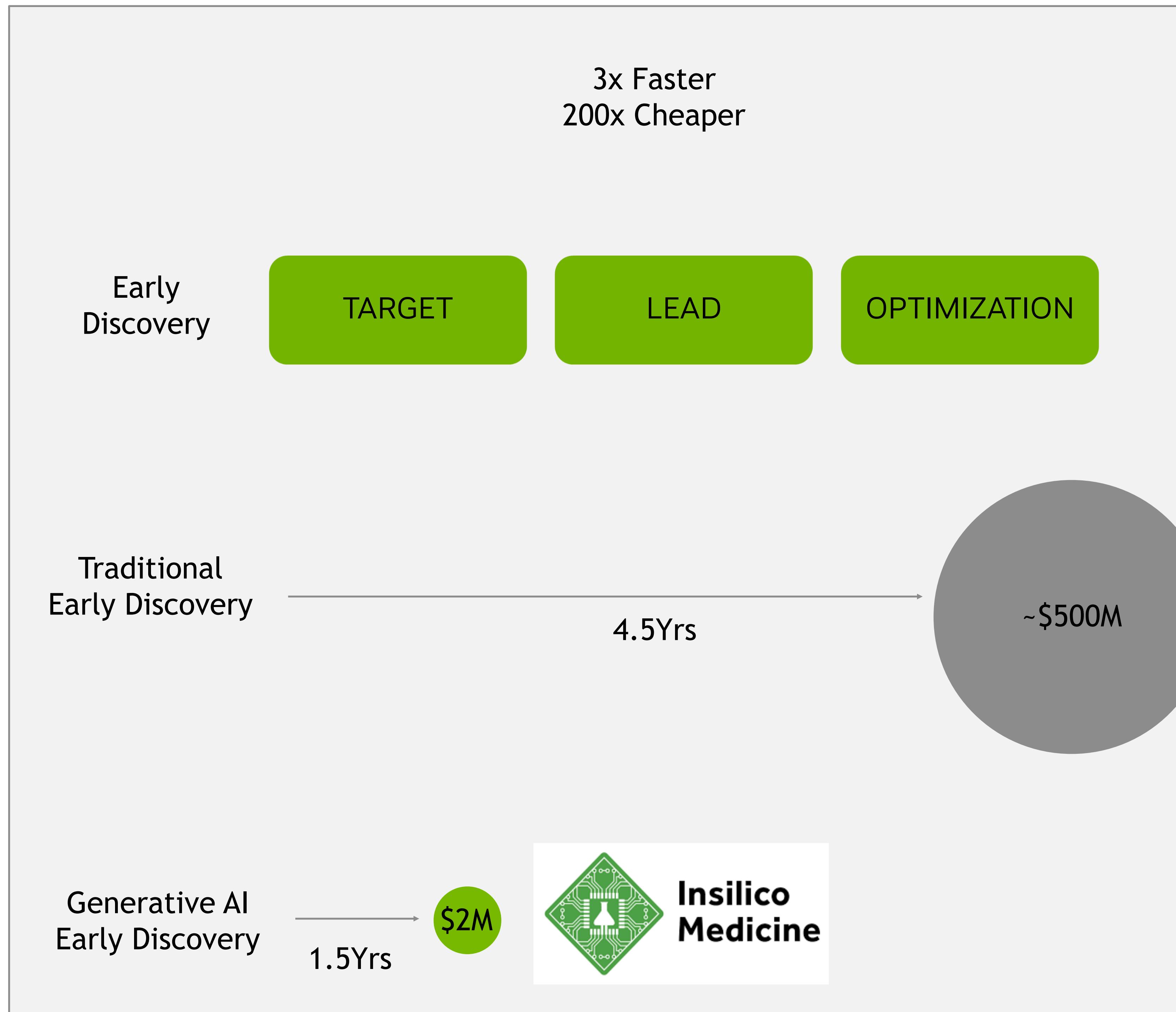
Models for AI-Powered Virtual Screening

DiffDock | Pose Prediction Significantly Exceeding State-of-the-Art Methods



Insilico Medicine: Generative AI is Accelerating Early Drug Discovery

Generative AI Early Discovery

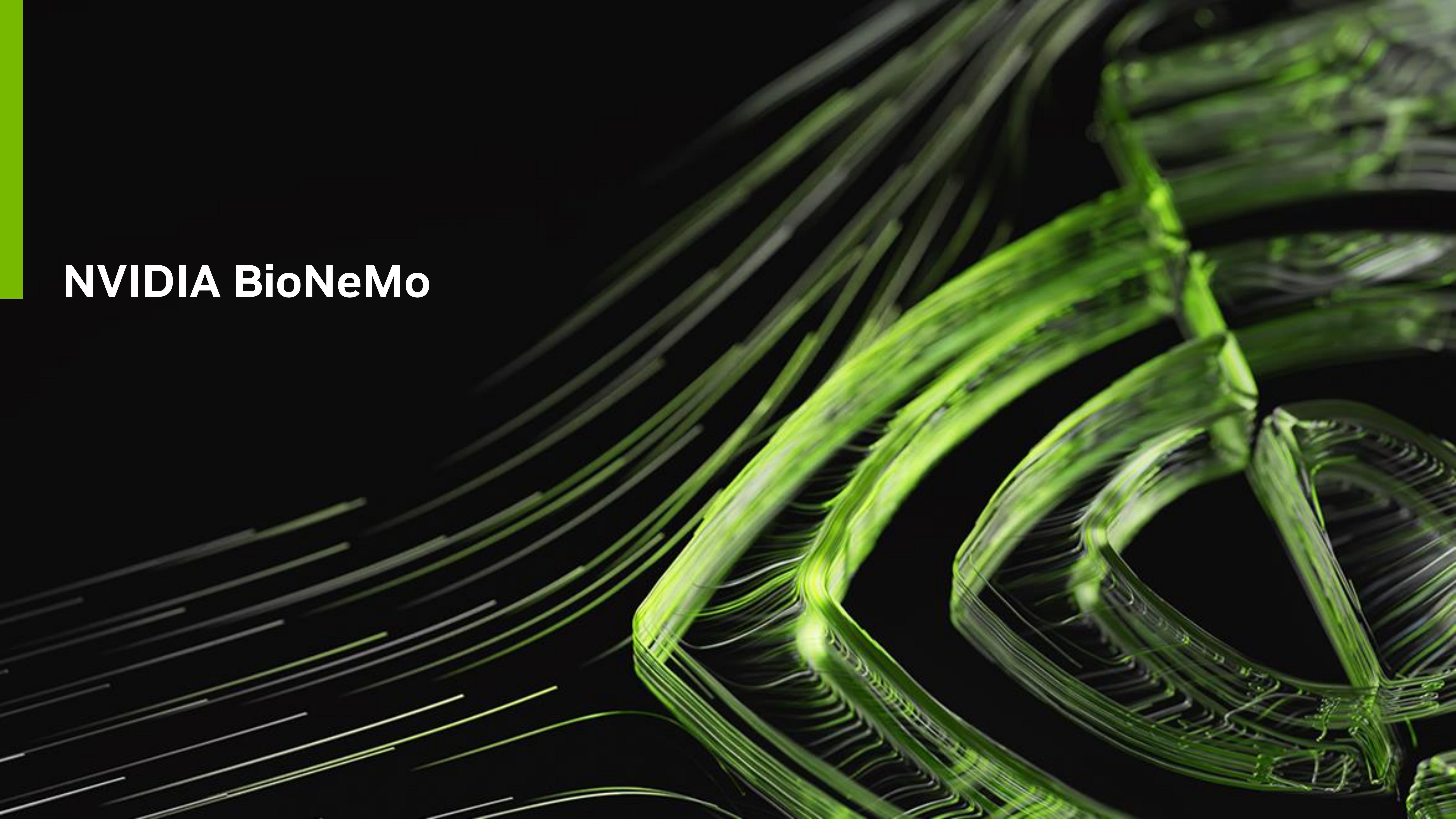


The screenshot shows a news release from EurekAlert! dated February 8, 2023, from AAAS.

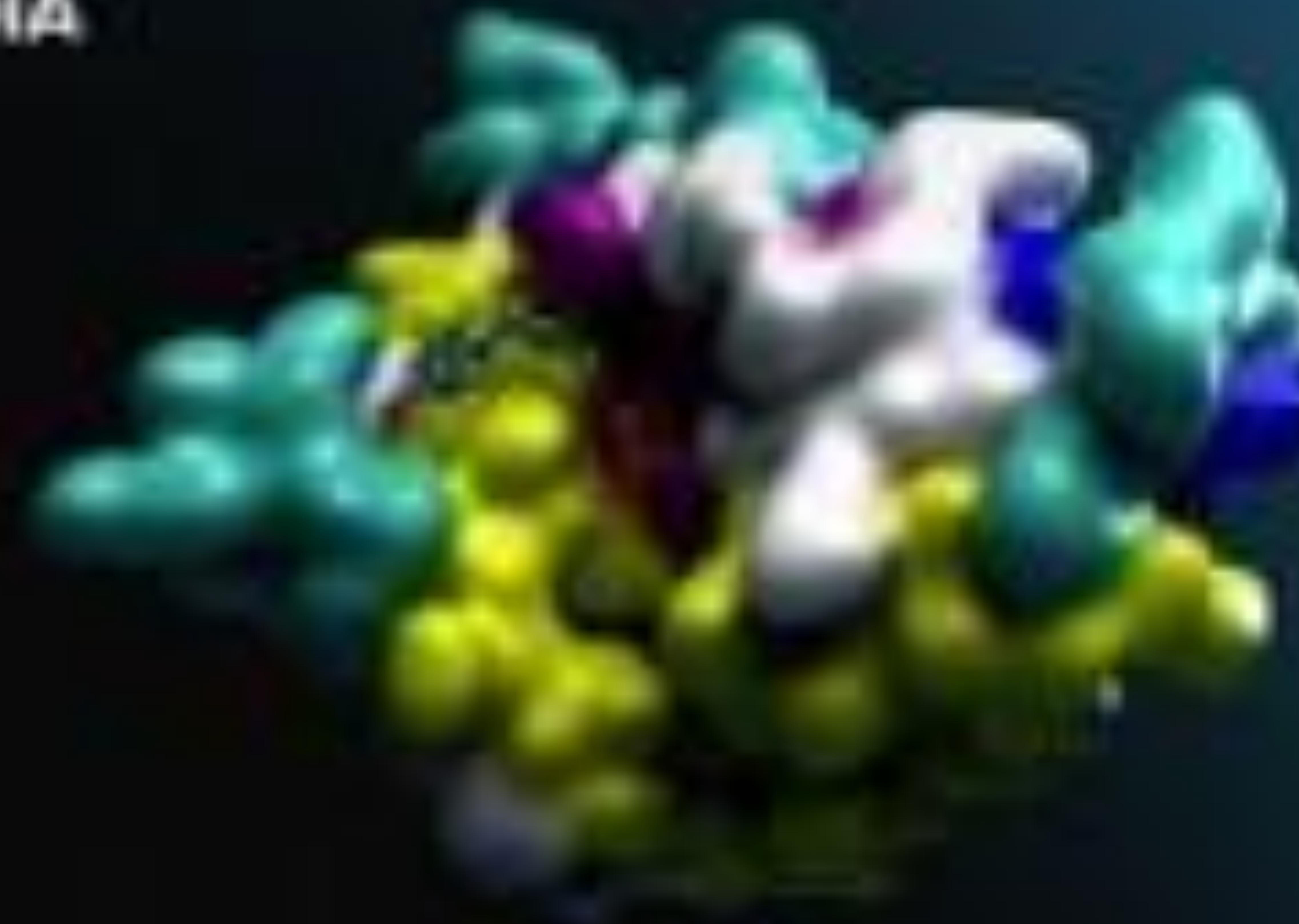
News Release: Insilico Medicine receives FDA Orphan Drug Designation for generative AI discovered and designed drug for idiopathic pulmonary fibrosis

Business Announcement: INSILICO MEDICINE

<https://www.eurekalert.org/news-releases/979045>



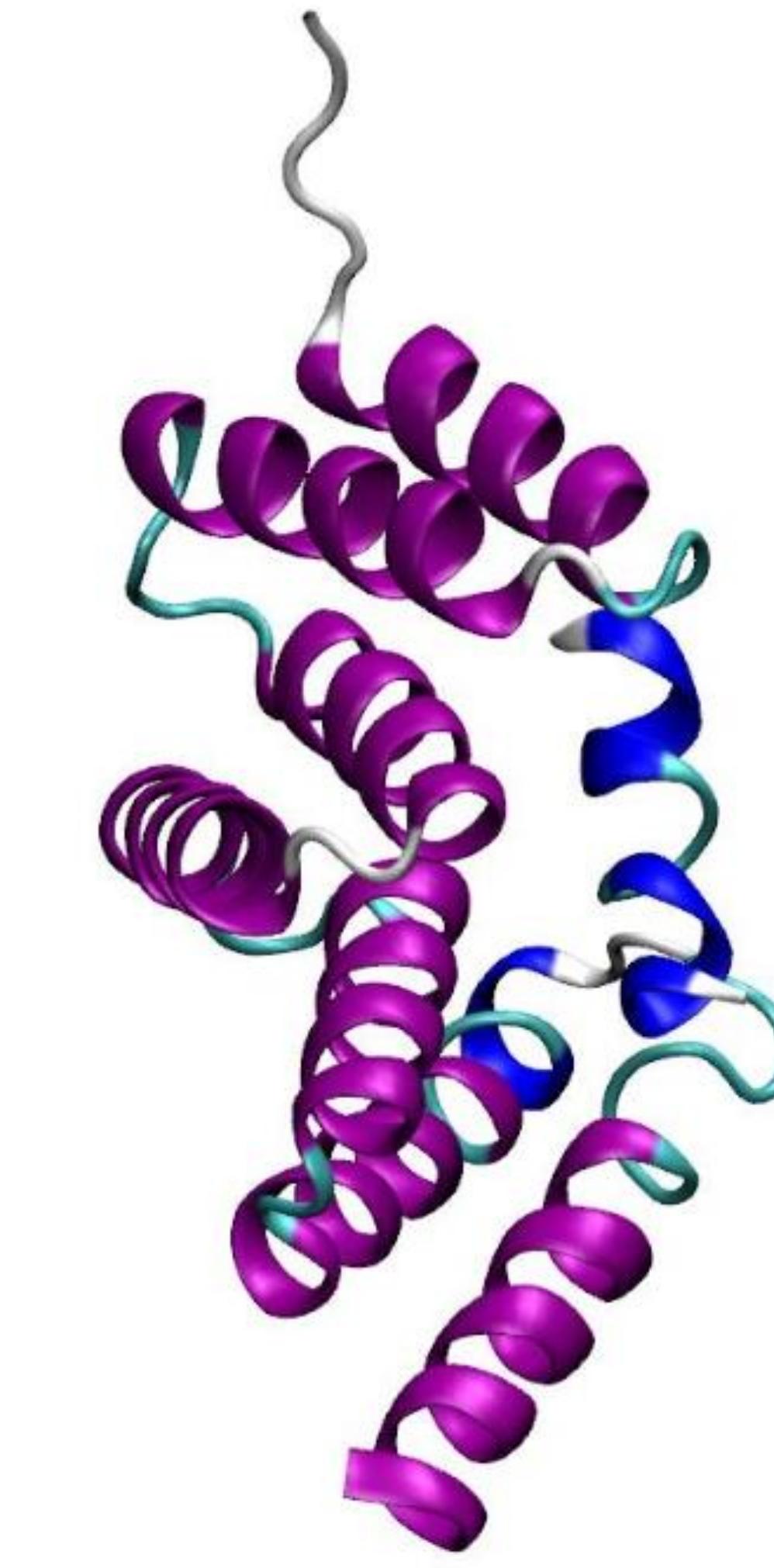
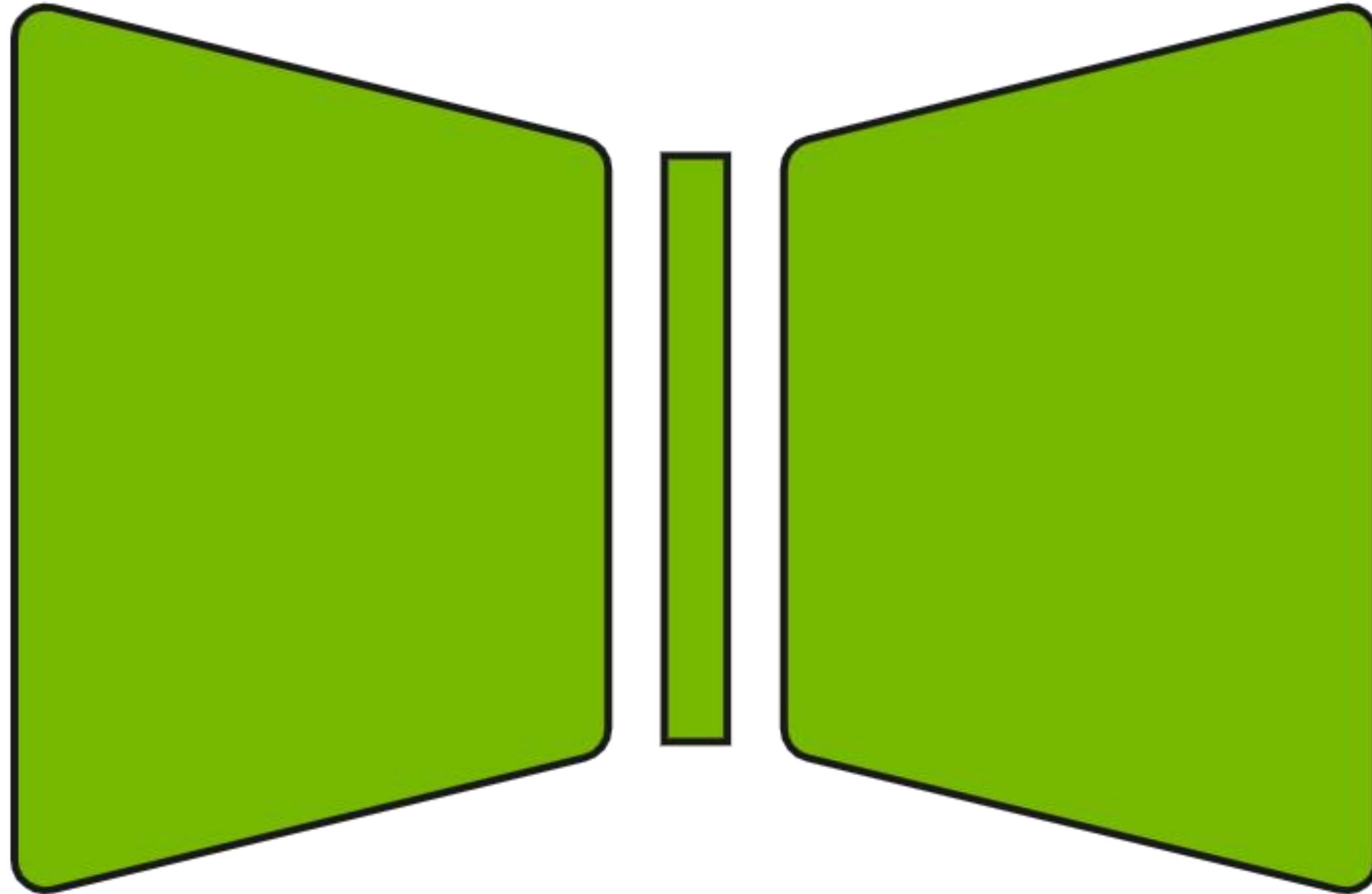
NVIDIA BioNeMo



BioNeMo – Protein Structure Prediction

AlphaFold2, OpenFold, ESMFold | Fold Proteins with BYO MSA or MSA-Free

MHHHHHSSGLVPRGSGMKGETAAAKFERQH
MDSPDLGTTDDDKAMADIGSENLYFQSMSK
IFVNPSAIRAGMADLEMAEETVDLINRNIE
DNQAHLQGEPIEVDSLPEDEIENLYFQGMES
DKIVFKVNNNQLVSVKPEVIVDQYEYKYPAI
QDHHTKPSITI GKAPDIINKAYKSTI SGMNAA
KLDPDDVCSYLAAMELFEGVCPEDWTSYG
IMIARKGDKITPATLVDIKRTDIEGNWALT
GGQDLTRDPTVAEHASLVGLLILSLYRLSKI
SGQNTGNYKTNIADRIEQIFETAPFAKIVE
HHTLMTTHKMCANWSTIPNFRFLAGTYDMF
FSRVEHLYSAIRVGTVVTAYEDCSGLVSFT
GFIKQIN



AlphaFold-2: DeepMind; Jumper et al.

RoseTTAFold: UW IPD; Baker et al.

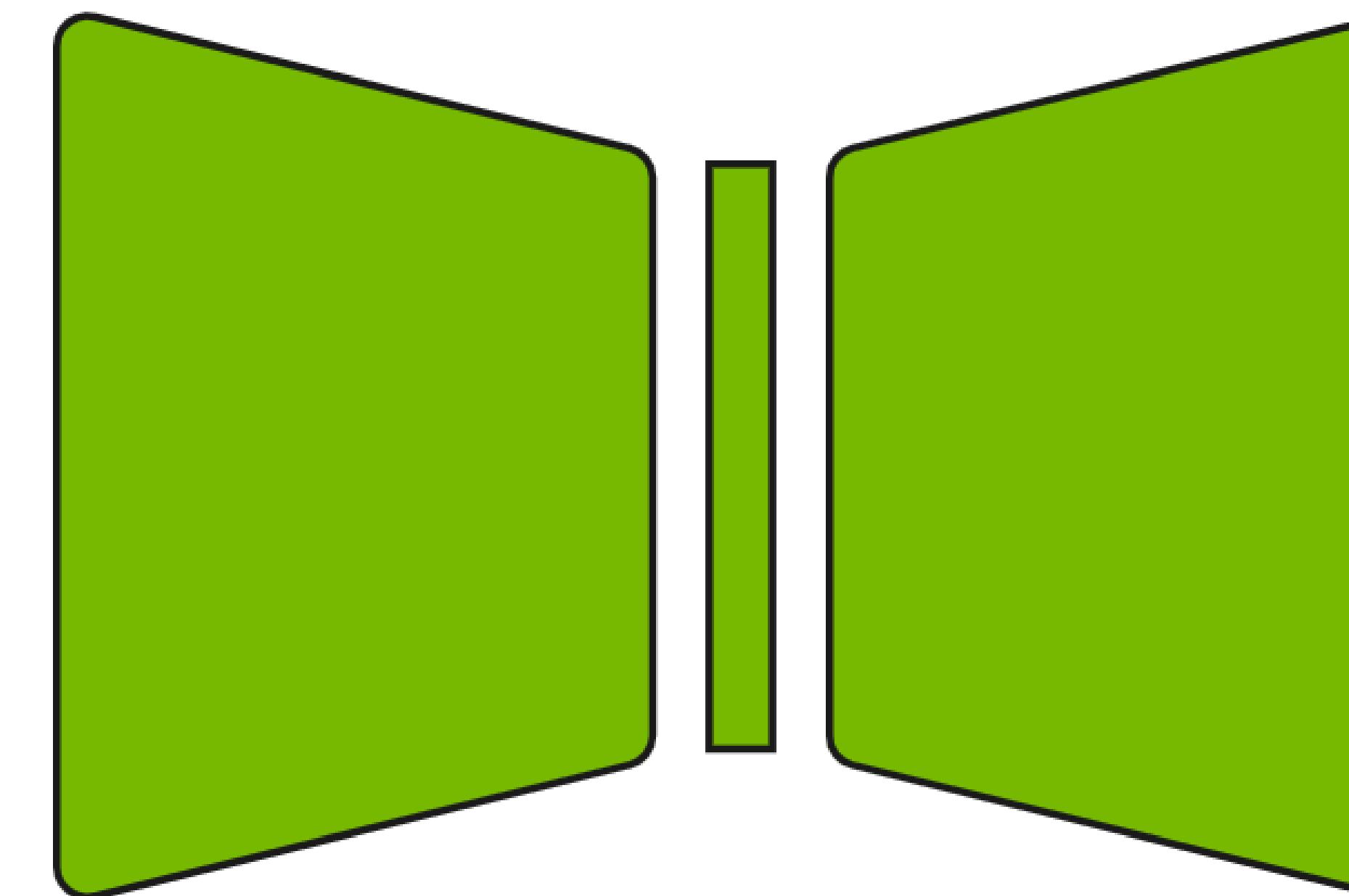
OpenFold: OpenFold Consortium; AlQuraishi et al.

ESMFold: MetaAI; Lin et al.

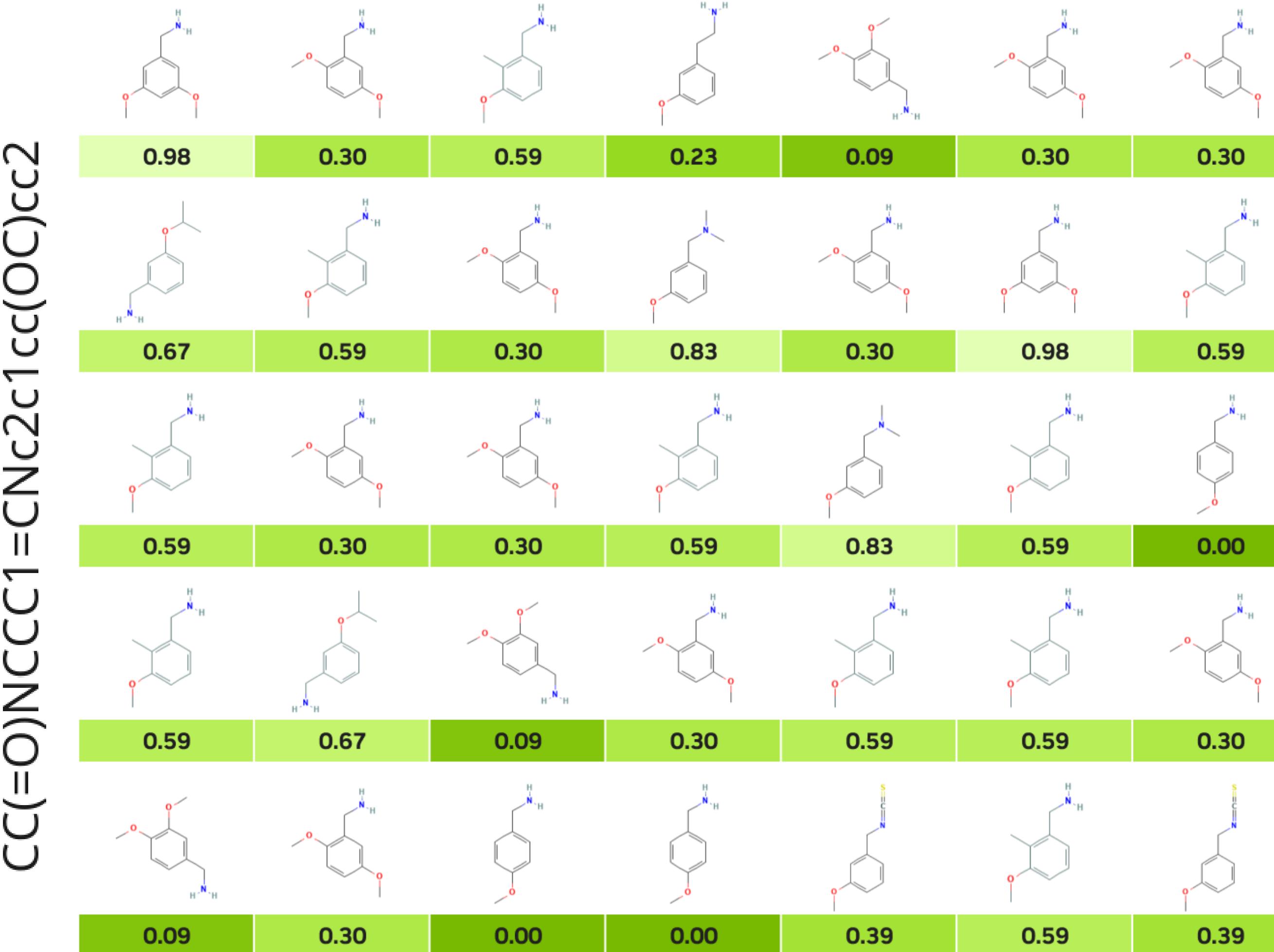
BioNeMo – Molecule Generation

MoFlow & MegaMolBART | Generate Molecules with Optimized Properties

COc(c1)cccc1CN



CC(=O)NCCCC1=CNc2c1cc(OC)cc2



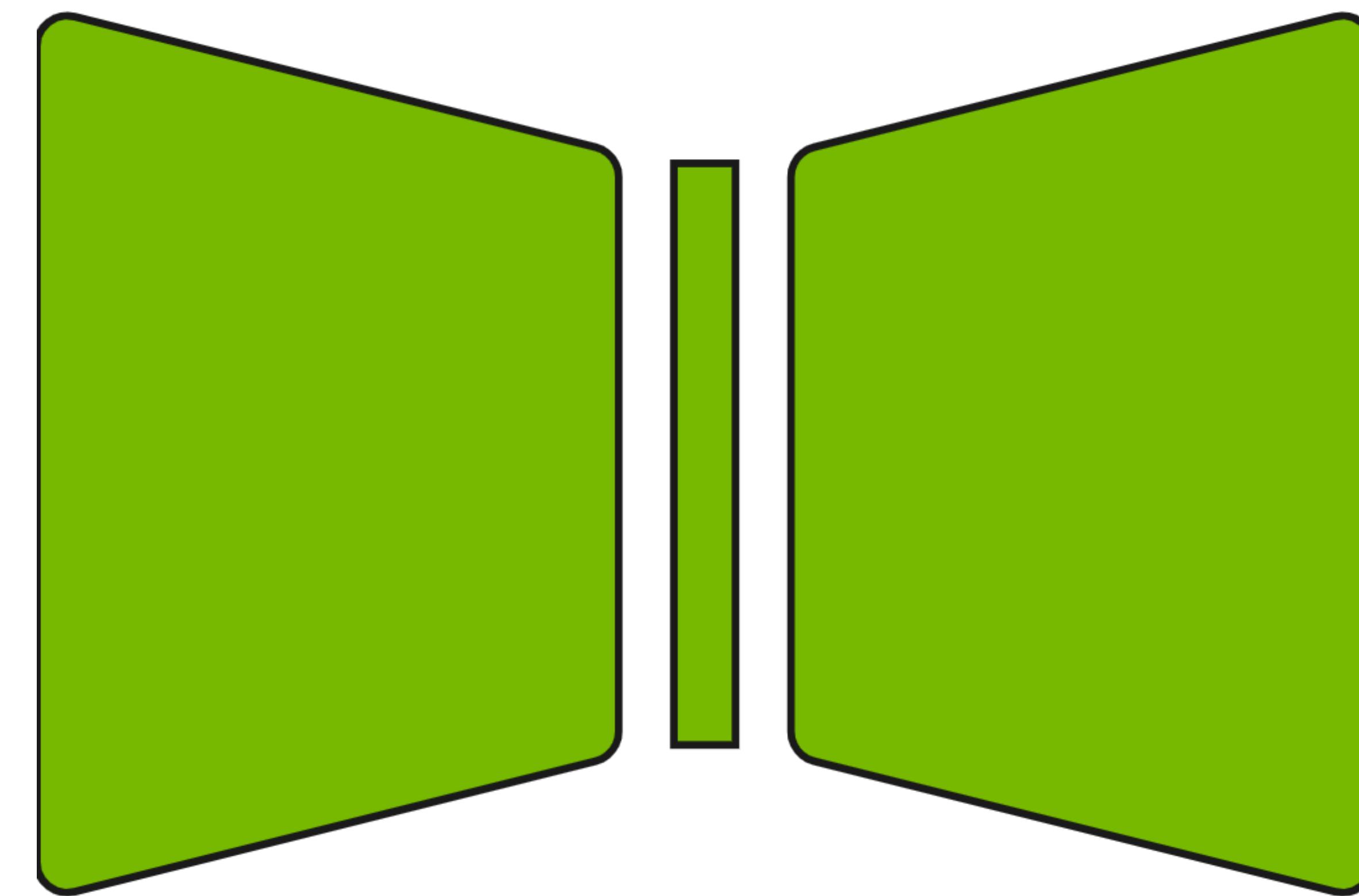
MoFlow: Chengxi Zang and Fei Wang

MegaMolBART: NVIDIA & AstraZeneca; Bjerrum, Irvin, Engkvist, et al.

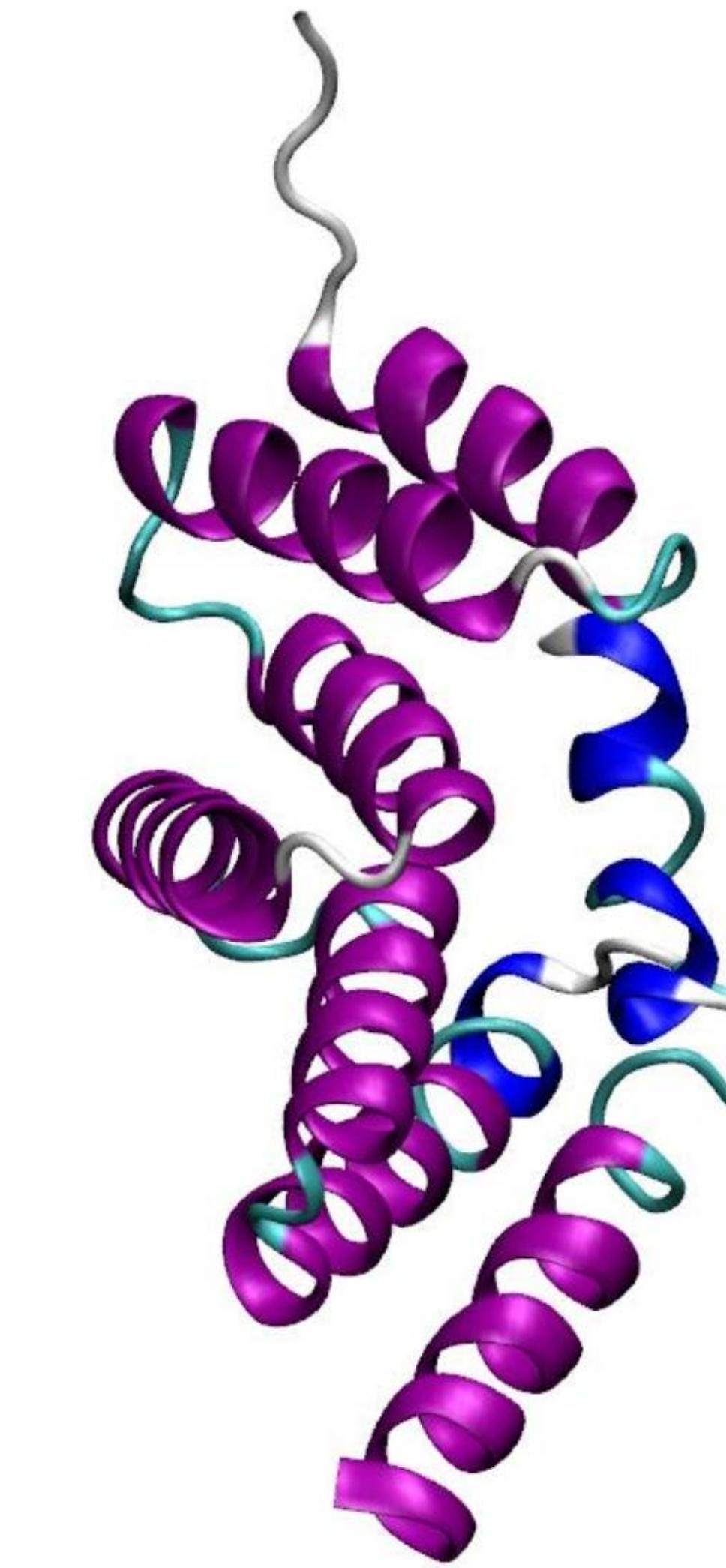


Protein Sequence Generation

ProtGPT2



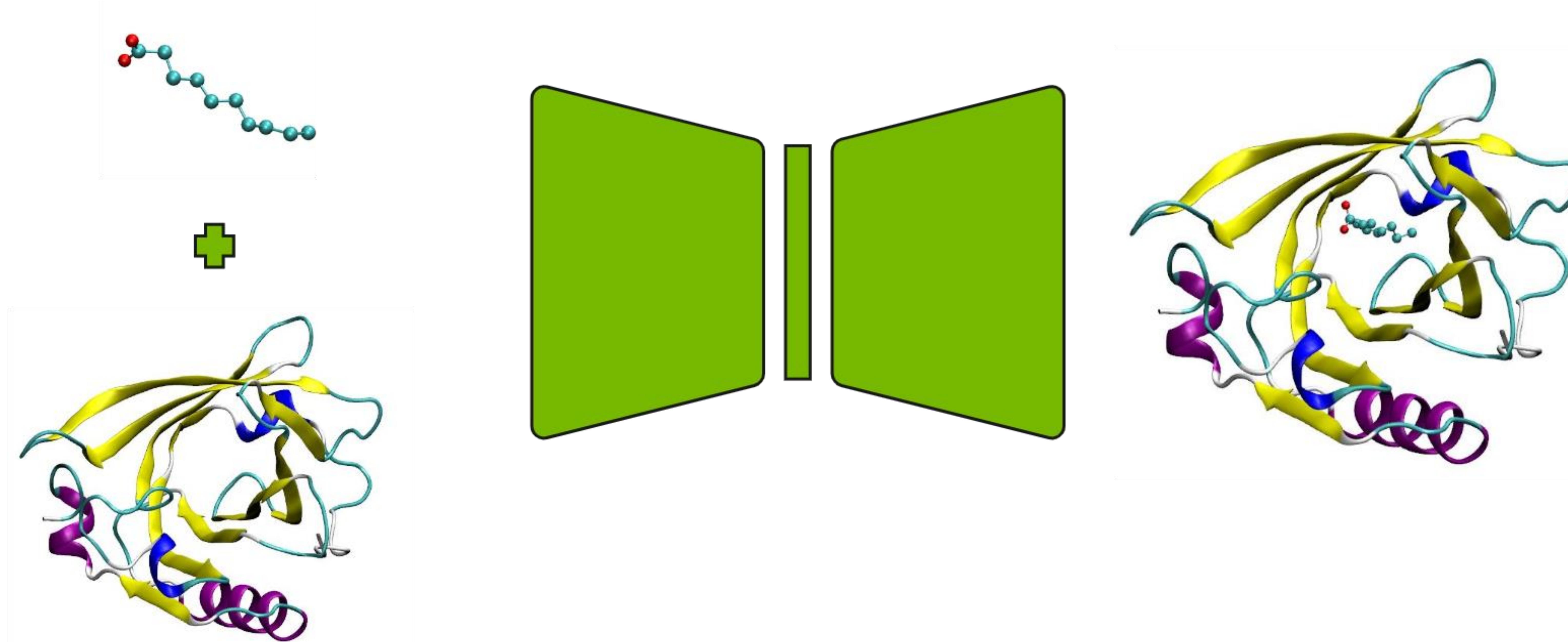
MHHHHHSSGLVPRGSGMKGTEAAAKFERQHQMDSPDL
GTDDDKAMADIGSENLYFQSMSKIFVNPSAIRAGM
ADLEMAEETVDLILNRNIEDNQAHLQGEPIEVDSLPE
DIENLYFQGMESDKIVFKVNINQLVSVKPEVIVD...



miro

BioNeMo – Docking Pose Prediction

DiffDock | Pose Prediction Significantly Exceeding State-of-the-Art Methods

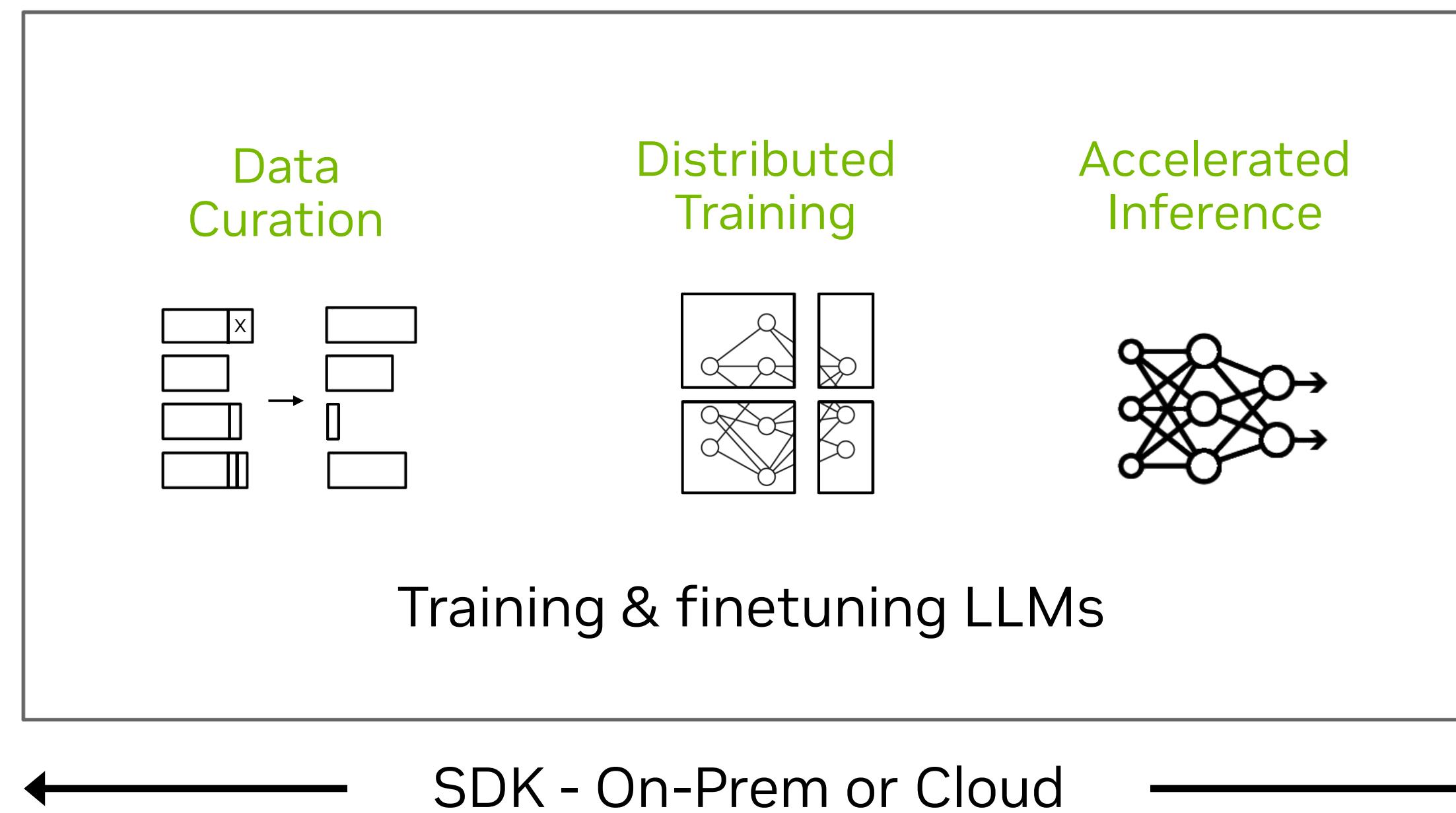


38% top-1 success rate (RMSD<2A) on PDB-Bind

Gabriele Corso, Hannes Stark, Bowen Jing, Regina Barzilay & Tommi J

NVIDIA BioNeMo Framework / Service

BioNeMo Training



AI Models in BioNeMo

- MegaMolBART is LLM for state-of-the-art **small molecule generation**
- MoFlow is for **generative chemistry**
- ESM1nv is LLM for **protein embeddings** for downstream tasks
- ESM2 is LLM for **protein embeddings** for downstream tasks
- ProtGPT2 is for **protein generation**
- DiffDock is for molecular **docking pose estimation**

Domain Specific

Drug discovery researchers need an LLM framework that speaks the language of biology and chemistry.

Optimized For Scale

LLMs are massive requiring model parallelism and supercomputing resources to train.

Pre-Trained Models

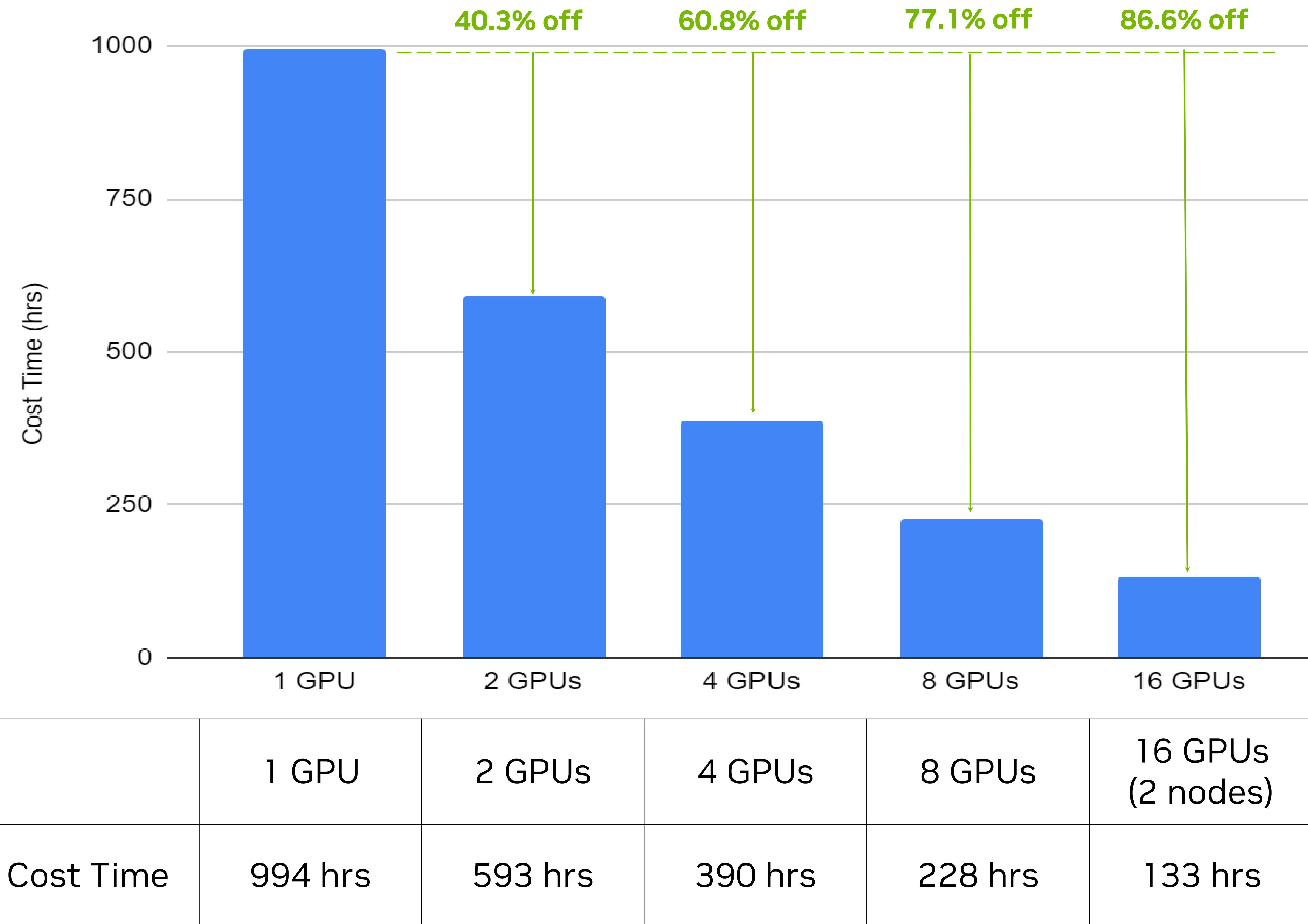
Training LLMs takes enormous compute resources and is very time consuming. Pre-trained models are ready for production.

Cloud Native

Use pre-trained models, create powerful customized workflows and deploy in the cloud.

Language Model Multi-GPU Benchmarking

Model = 384m parameters, Data = 6B protein sequences, Machine: DGX A100



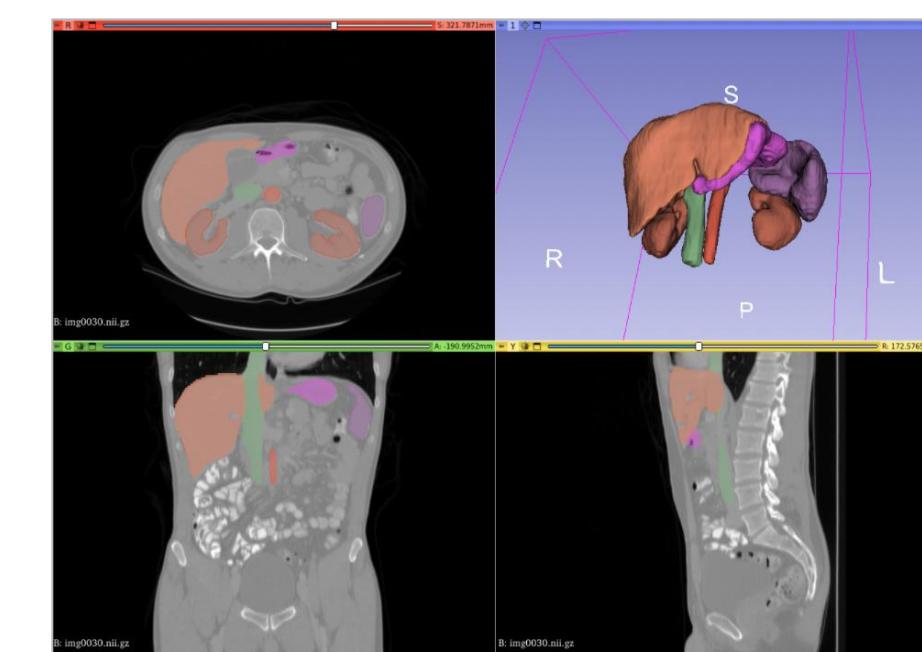


MONAI Generative AI

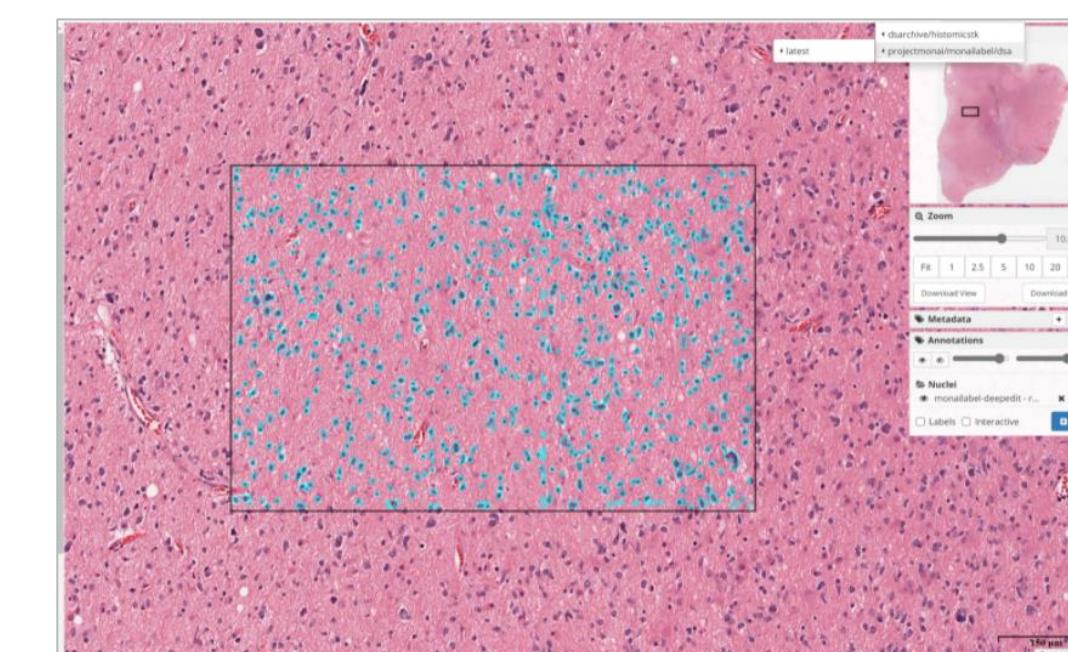
MONAI

Industry Standard Medical AI Framework

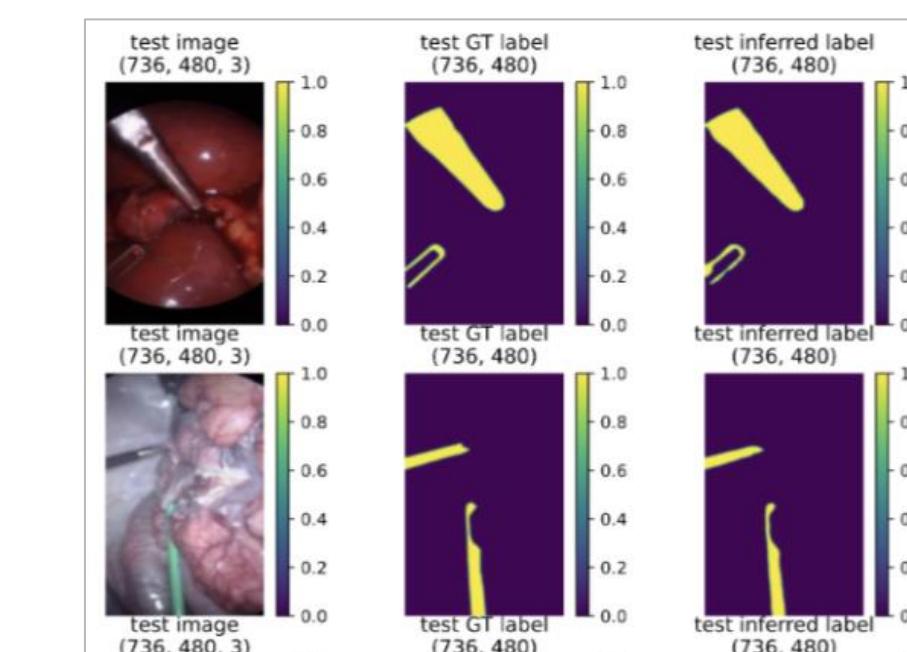
MONAI



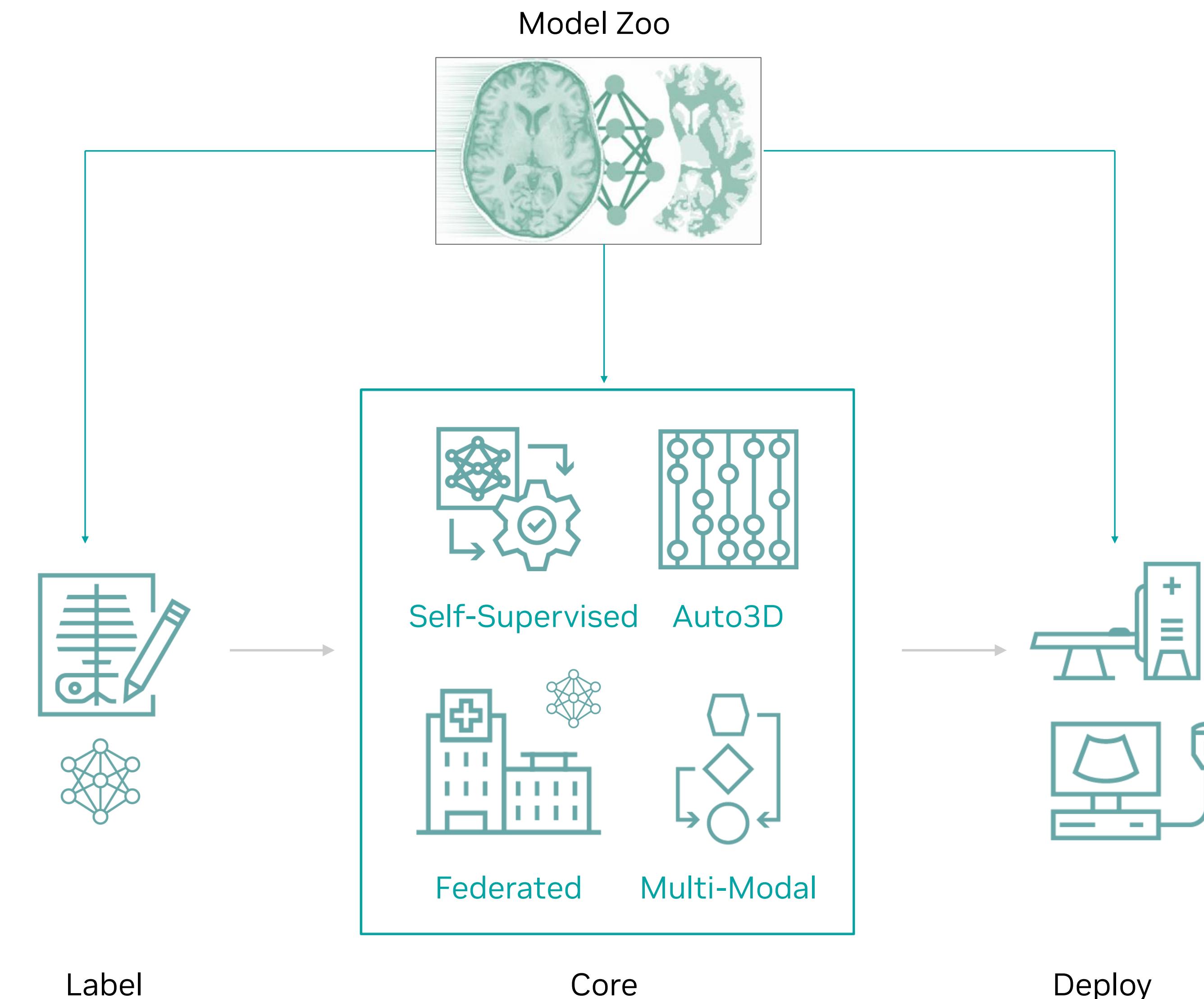
Radiology



Pathology

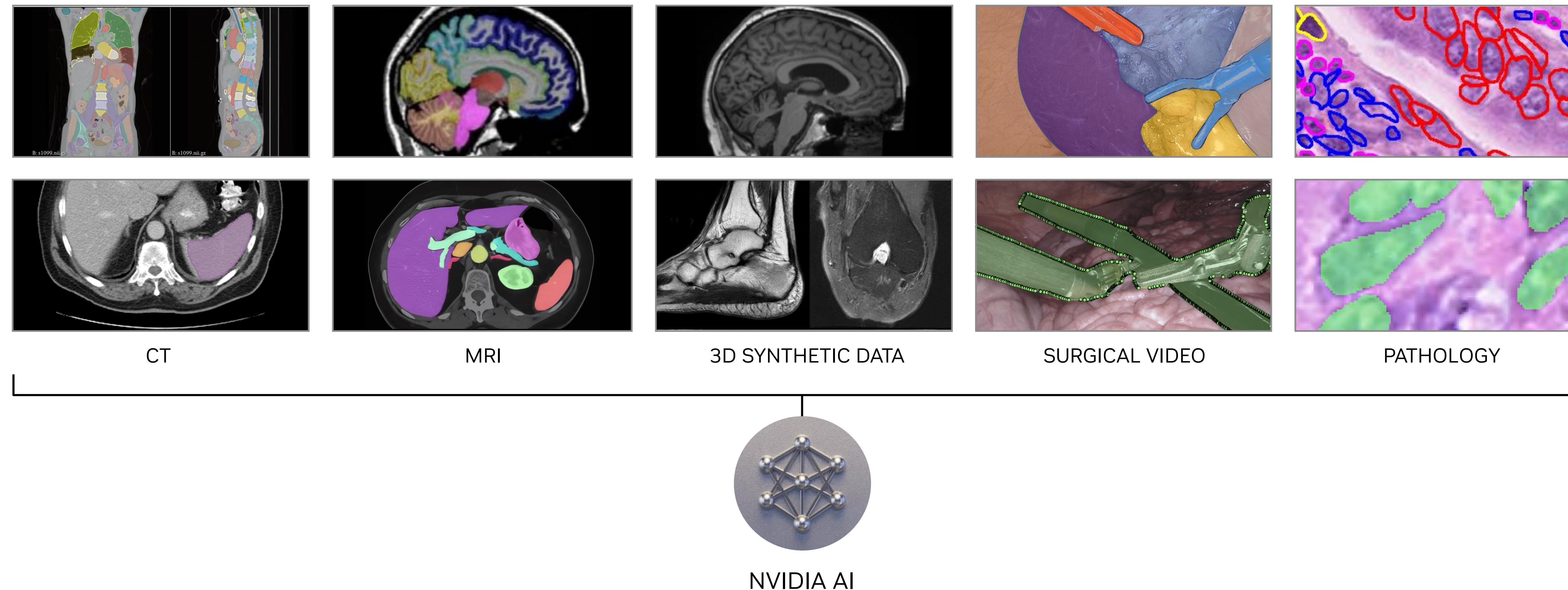


Endoscopy



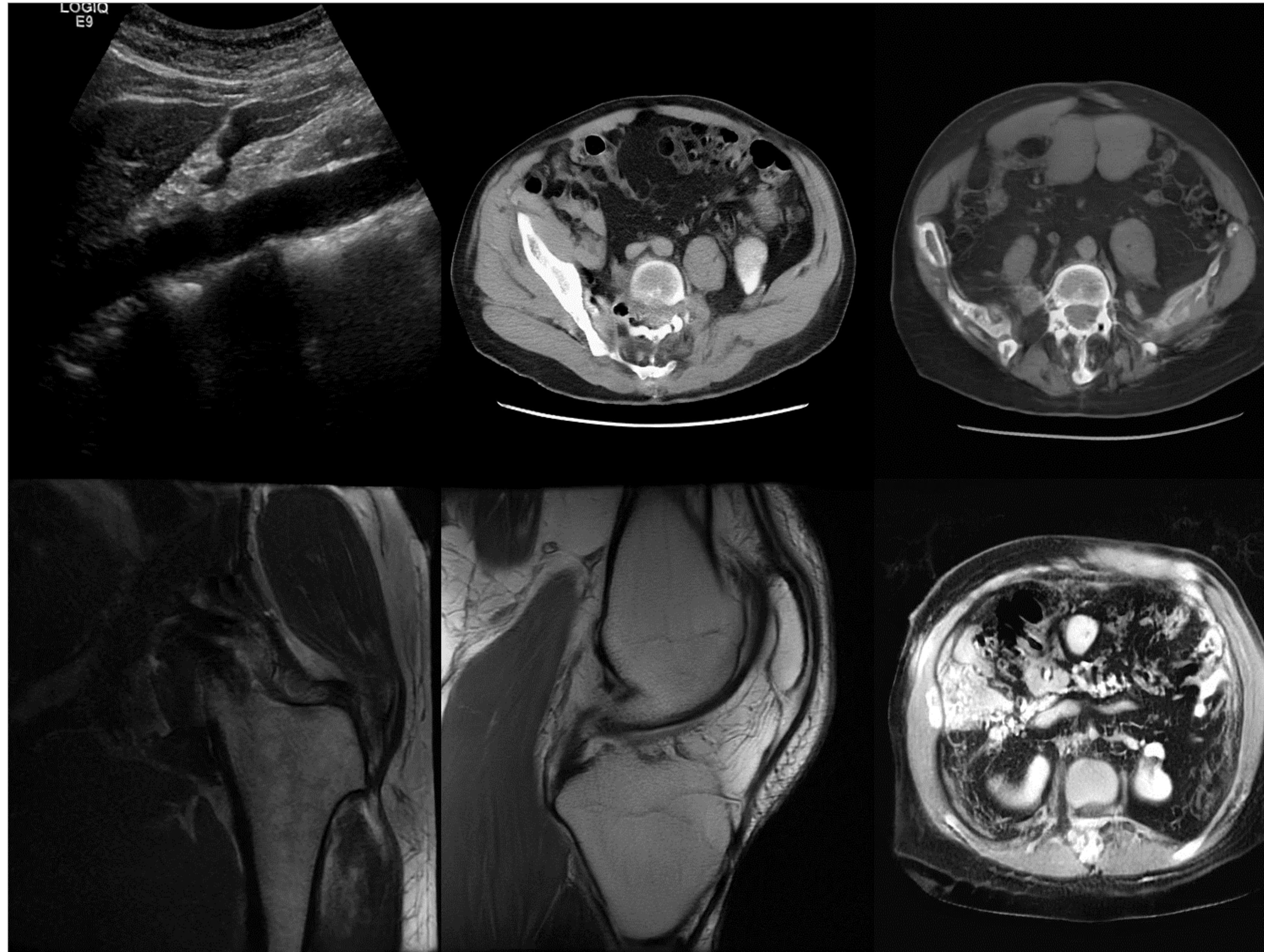
MONAI Model Zoo

Plug Into Any MONAI Workflow from Labeling to Training to Deployment



MONAI Generative AI

Create Infinite Medical Imaging Data with Generative AI



RADIMAGEGAN

3 modalities CT, MRI, US, 14 anatomies, and 165 pathologic labels

NVIDIA | Mt. Sinai | East River Imaging

Available NGC Catalog

Generating Brain Imaging with Diffusion Models

Inputs

Gender: Male

Age [years]: 68

Volume of ventricular cerebrospinal fluid: 0.39

Volume of brain: 0.59

Generate

Axial View Sagittal View Coronal View

My Brain my_brain.nii.gz 4.4 MB Download

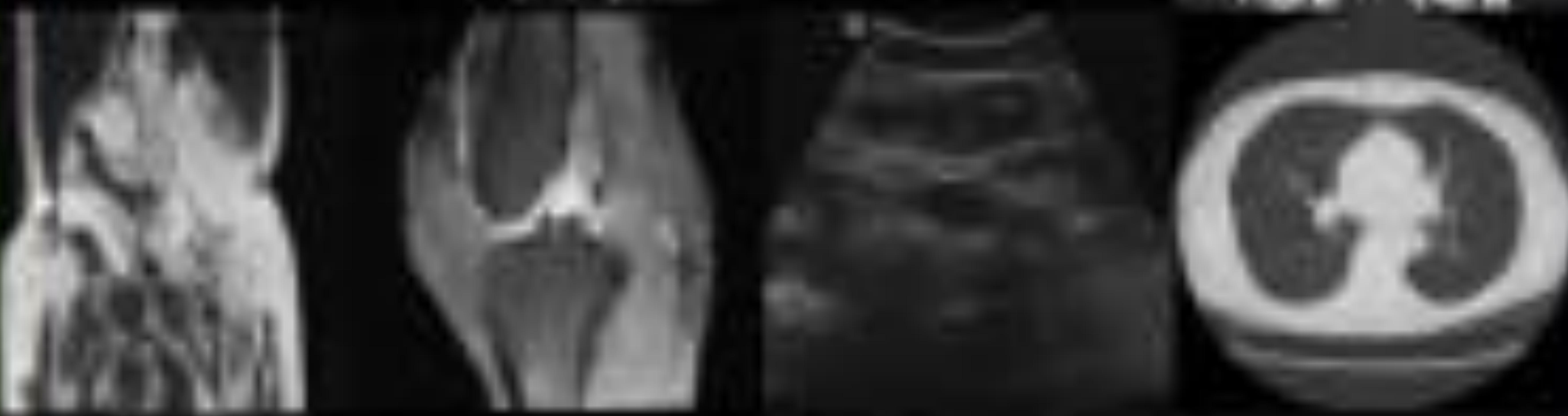
Use via API · Built with Gradio

Latent Diffusion Model

High-resolution brain images | Targeted datasets for brain volume, age, disease

NVIDIA | Kings College London

Available NGC Catalog | MONAI Model Zoo



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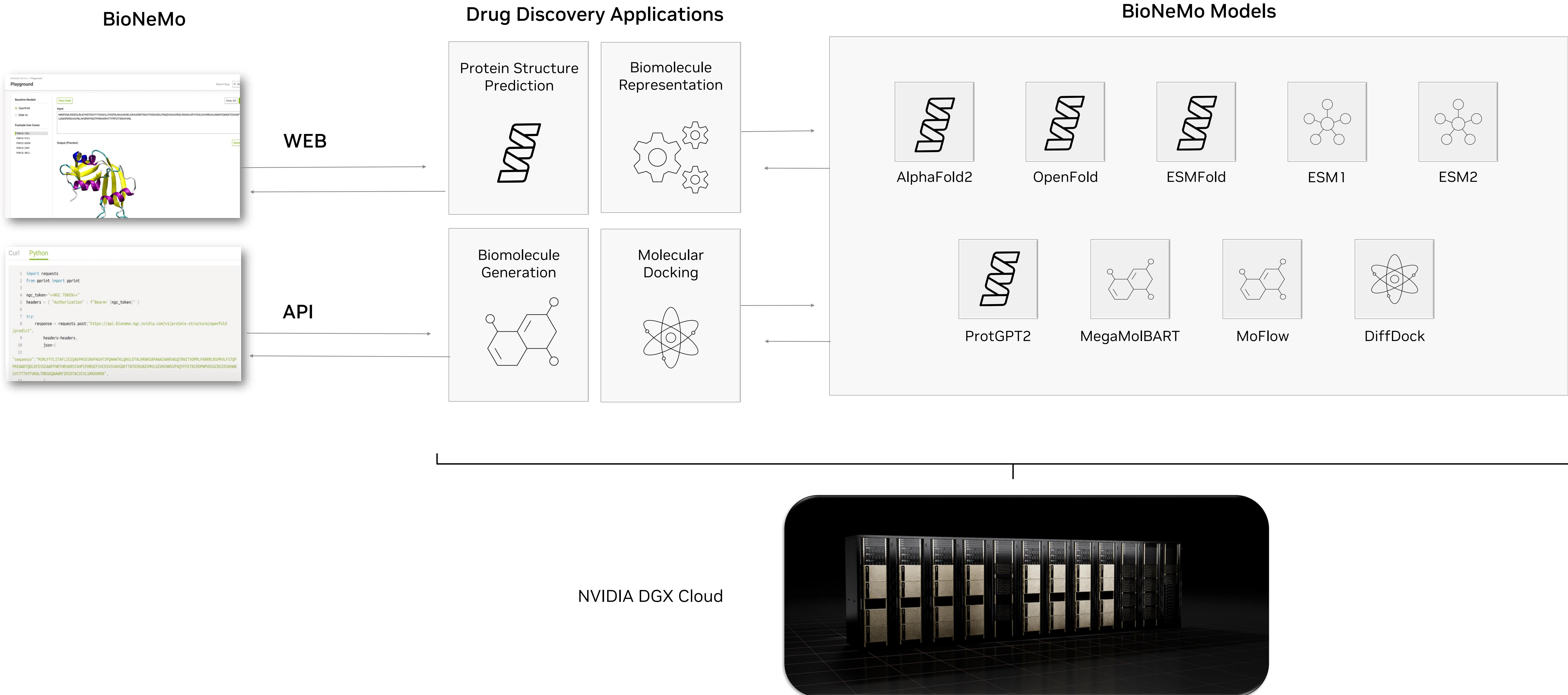


Thank You



BioNeMo

For Generative AI in Biology - Supporting 9 SOTA Small Molecule & Protein AI Models at HPC Scale



NVIDIA GPU Cloud

Free to register and download

 NVIDIA NGC | CATALOG

Welcome Guest ▾

CATALOG

- Explore Catalog
- Collections
- Containers
- Helm Charts
- Models**
- Resources

Catalog > Models

Models

The NGC catalog offers 100s of pre-trained models for computer vision, speech, recommendation, and more. Bring AI faster to market by using these models as-is or quickly build proprietary models with a fraction of your custom data.

monai

Sort: Relevance

Displaying 9 results

	MONAI ⁺	MONAI ⁺	MONAI ⁺
MONAI BraTS MRI Segmentation	A pre-trained model for volumetric (3D) segmentation of brain tumor subregions from multimodal MRIs based on BraTS 2018 data.	MONAI Endoscopic Inbody Classification	MONAI Endoscopic Tool Segmentation
	View Labels Download	View Labels Download	View Labels Download

NVIDIA AI Enterprise Support

Yes 9

Use Case No results found

NVIDIA Platform No results found

Framework

Industry

Solution

?

<< Collapse

NGC Catalog v1.56.17



MONAI Gen AI Official GitHub

<https://github.com/Project-MONAI/GenerativeModels>

Product ▾ Solutions ▾ Open Source ▾ Pricing Search / Sign in Sign up

Project-MONAI / GenerativeModels Public Notifications Fork 16 Star 174

Code Issues 39 Pull requests 10 Discussions Actions Projects Security Insights

main 28 branches 1 tag Go to file Code

Warvito Add figure (#370) ...	b4c66b7 2 days ago	388 commits
generative	Adopt original computation of FID (#355)	last week
model-zoo	Add figure (#370)	2 days ago
tests	Fix typo (#367)	3 days ago
tutorials	Fix number of attention heads (#369)	2 days ago
.depsource.toml	Update tests, CI and pre-commit (#193)	3 months ago
.gitignore	Modified .gitignore to account for all IteliJ tools.	6 months ago
.pre-commit-config.yaml	Change num_res_channels and num_channels to Sequence[int] int (#237)	2 months ago
CODE_OF_CONDUCT.md	Create CODE_OF_CONDUCT.md	5 months ago
CONTRIBUTING.md	Refactor code with new pre commit configuration (#207)	3 months ago
LICENSE	Create LICENSE	5 months ago
README.md	Update README.md (#328)	3 weeks ago
pyproject.toml	Refactor code with new pre commit configuration (#207)	3 months ago
requirements-dev.txt	Add flash attention to Transformers (#342)	2 weeks ago

About

MONAI Generative Models makes it easy to train, evaluate, and deploy generative models and related applications

medical-imaging generative-adversarial-network

image-translation anomaly-detection

generative-models image-synthesis

mri-reconstruction diffusion-models

monai

Readme Apache-2.0 license

Code of conduct

174 stars 15 watching 16 forks

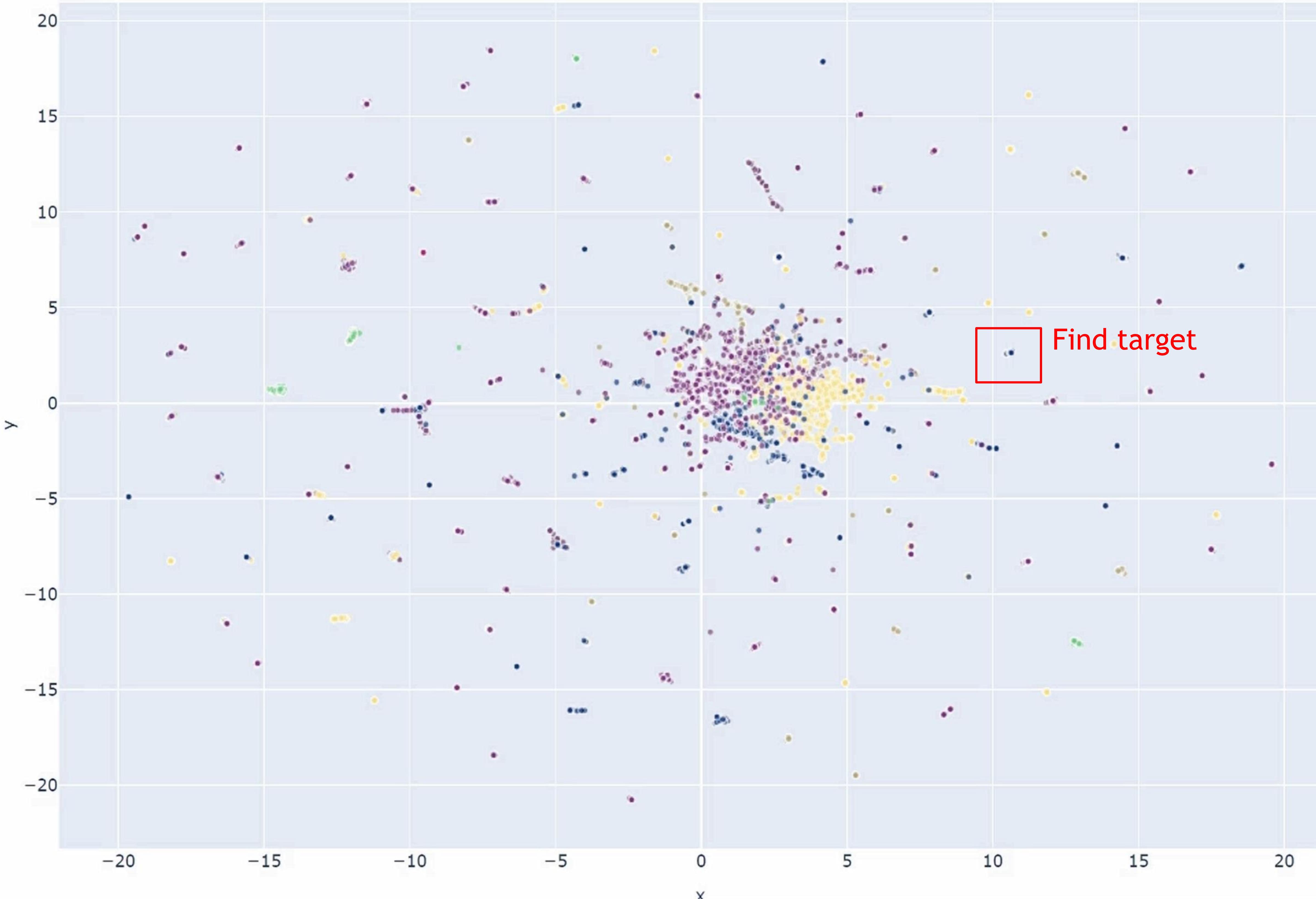
Report repository

Releases 1

Molecules Discovery Demo - MegaMolBART

<https://github.com/NVIDIA/cheminformatics>

Clusters



- Cluster 0
- Cluster 1
- Cluster 2
- Cluster 3
- Cluster 4
- Cluster 5
- Cluster 6

Molecule(s) of Interest

Please enter ChEMBL ID(s) separated by commas.

Highlight

Cluster Molecules	Generate Molecules
-------------------	--------------------

Select Workflow

GPU KMeans-UMAP

Apply

Cluster Selection

Set number of clusters

Click a point to select a cluster.

Recluster

Selection Points

Choose the lasso or rectangle tool in the graph's menu bar and then select points in the graph.

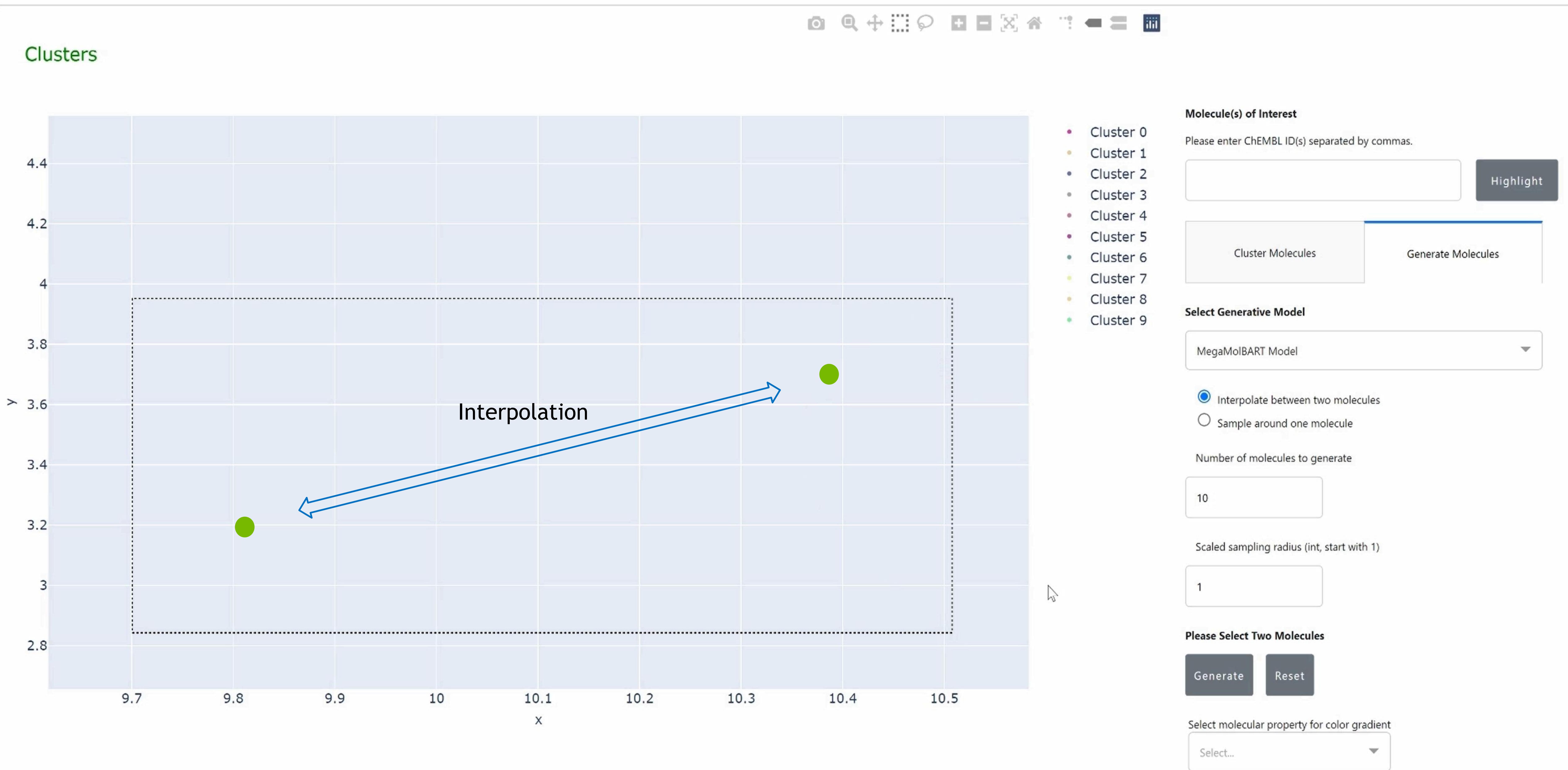
Recluster Selection

Reload

Select molecular property for color gradient

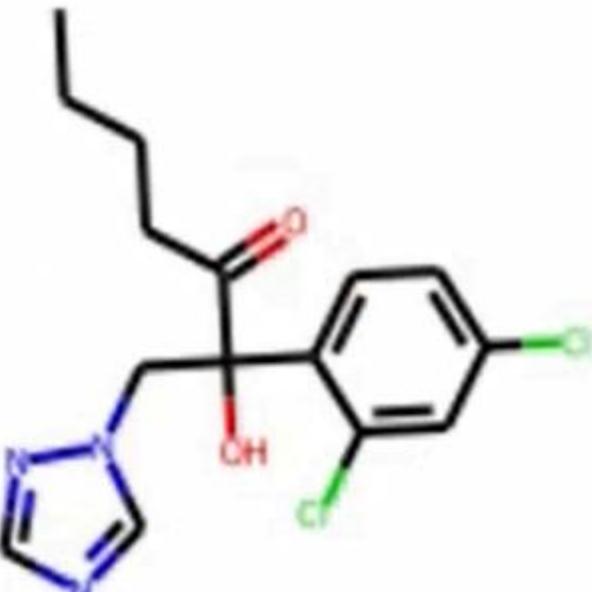
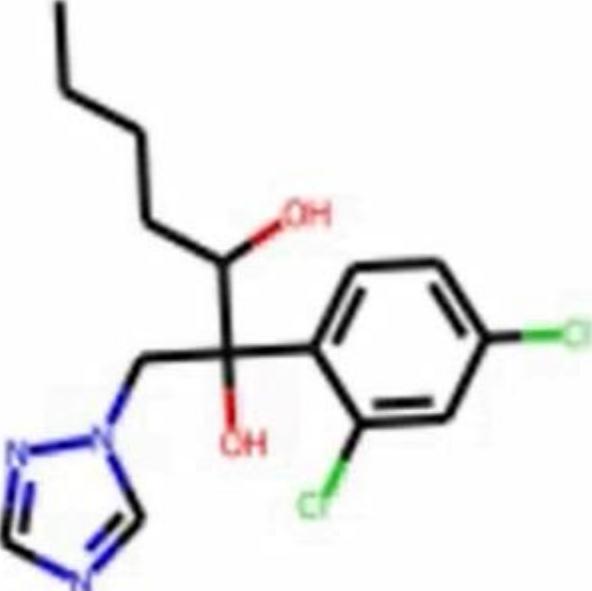
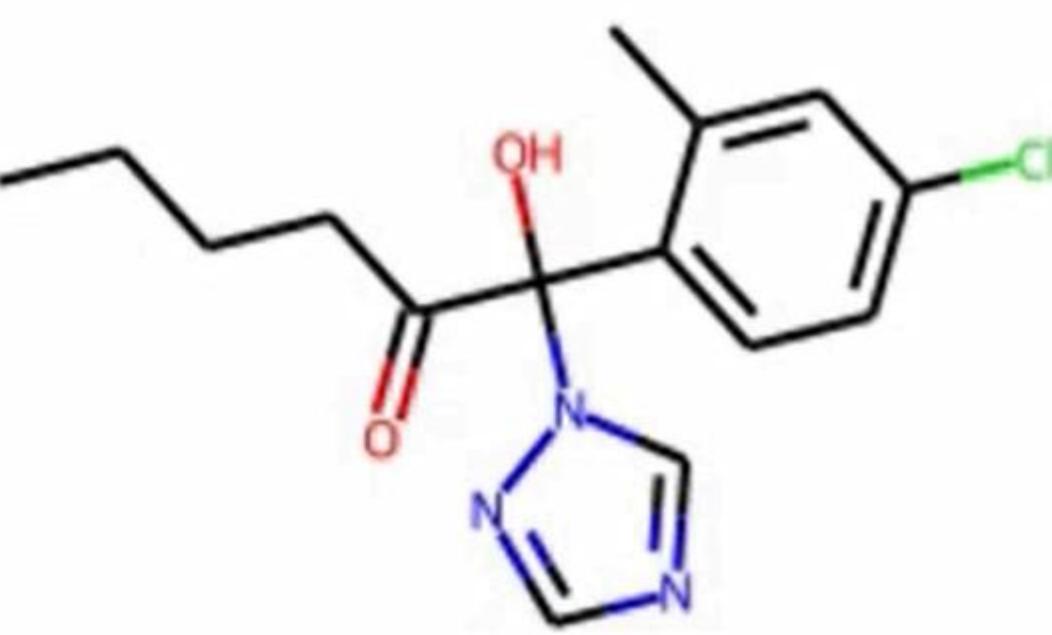
Molecules Discovery Demo - MegaMolBART

<https://github.com/NVIDIA/cheminformatics>



Molecules Discovery Demo - MegaMolBART

<https://github.com/NVIDIA/cheminformatics>

SMILES	Generated	Chemical Structure	Molecular Weight	LogP	H-Bond Donors	H-Bond Acceptors	Rotatable Bonds	QED
<chem>CCCCC(=O)C(O)(Cn1cncn1)c1ccc(Cl)cc1Cl</chem>	False		342.23	3.23	1	5	7	0.8388
<chem>CCCCC(O)C(O)(Cn1cncn1)c1ccc(Cl)cc1Cl</chem>	True		344.24	3.02	2	5	7	0.81
<chem>CCCCC(=O)C(O)(Cn1cncn1)c1ccc(Cl)cc1Cl</chem>	True		328.2	2.84	1	5	6	0.8853
<chem>CCCCC(=O)C(O)(n1cncn1)c1ccc(Cl)cc1C</chem>	True		307.78	2.69	1	5	6	0.8907