Ai DAY

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Agenda

Introduction and Vision

14:00	Welcome & Introductory Remarks
14:05	Our Vision for AI

Part I. Scaling AI Capabilities

14:10	Computing Infrastructure
14:25	Innovation: Bayesian Flow Networks
14:45	DeepChain: One Platform, Multiple Tools

Part II. Deploying AI across the pipeline

15:00	Applying AI end-to-end to the immunotherapy pipeline: examples
15:40	Closing Remarks and Q&A

Introduction and Welcome

Ugur Sahin
Founder & CEO
BioNTech

Ryan Richardson
Chief Strategy Officer
BioNTech

Karim Beguir
CEO
InstaDeep

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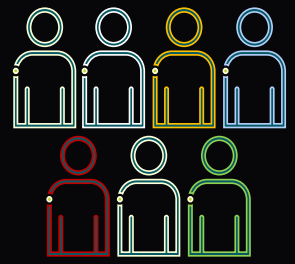
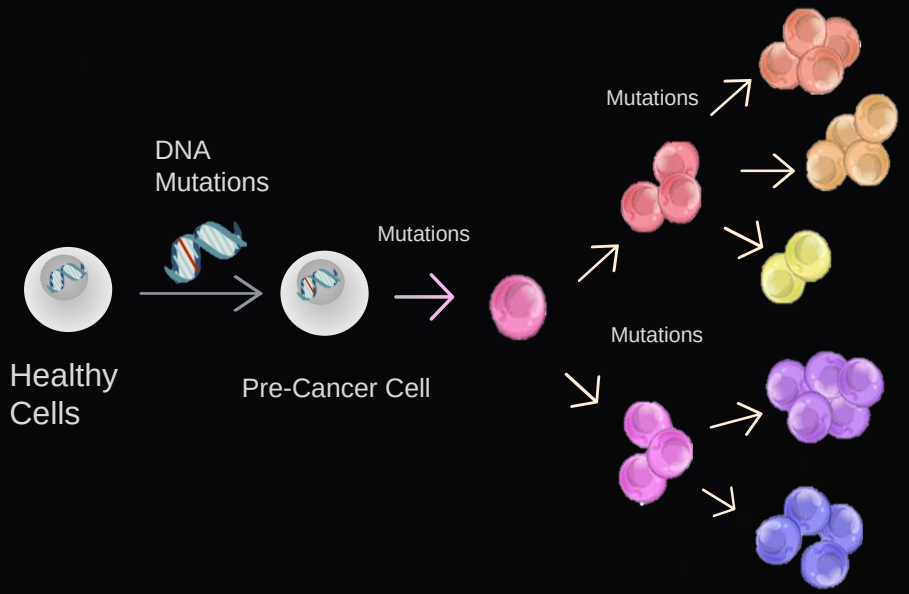
Root Cause of Cancer Treatment Failure

Interindividual Variability & Intratumoral Heterogeneity



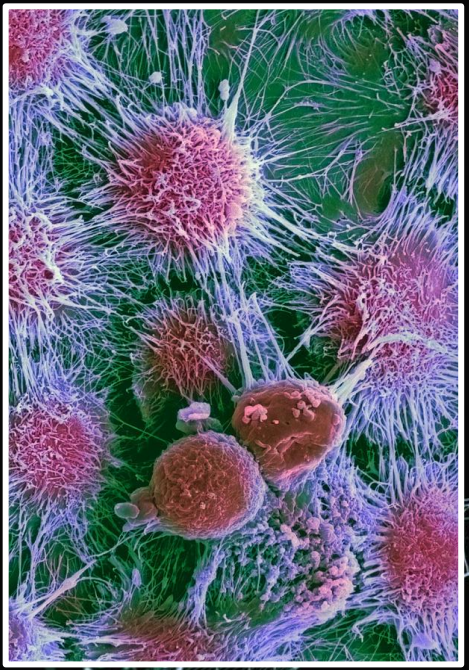
Individual Patients



Cancer Evolution 5-20 Years – up to 10.000 Mutations

Cancer Cells

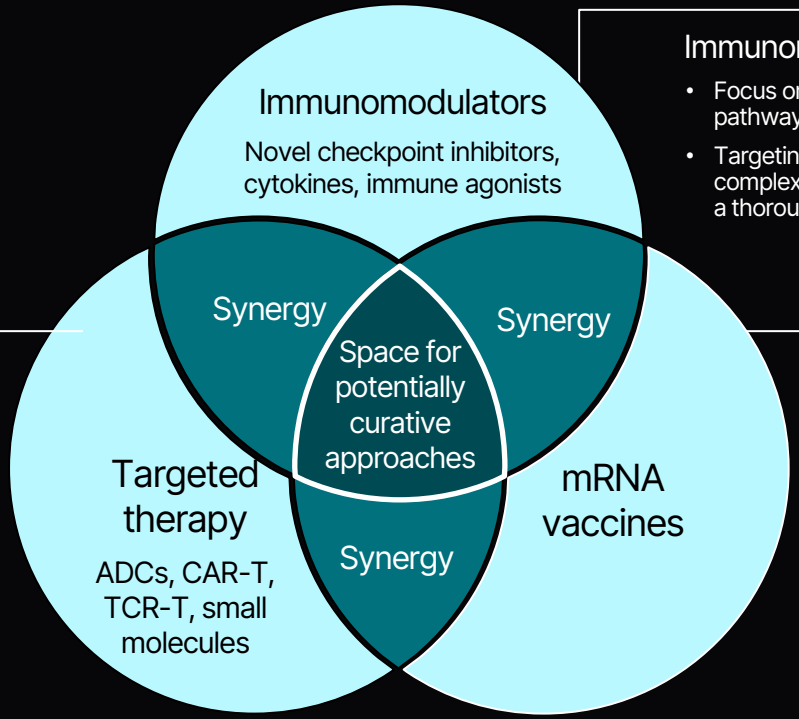
Genetically Diverse & Adaptable



Towards a Potentially Curative Approach to Cancer Based on Multiple Modalities and Differentiated Novel/Novel Therapeutic Combinations

Immunomodulators

- Focus on the most relevant and crucial IO pathways
- Targeting different complementary players in the complex cancer immunity cycle aiming to achieve a thorough and durable anti-tumor effect



Targeted therapy

- Could rapidly reduce tumor burden
- Designed with the aim to have clinical efficacy across the entire disease continuum including late lines

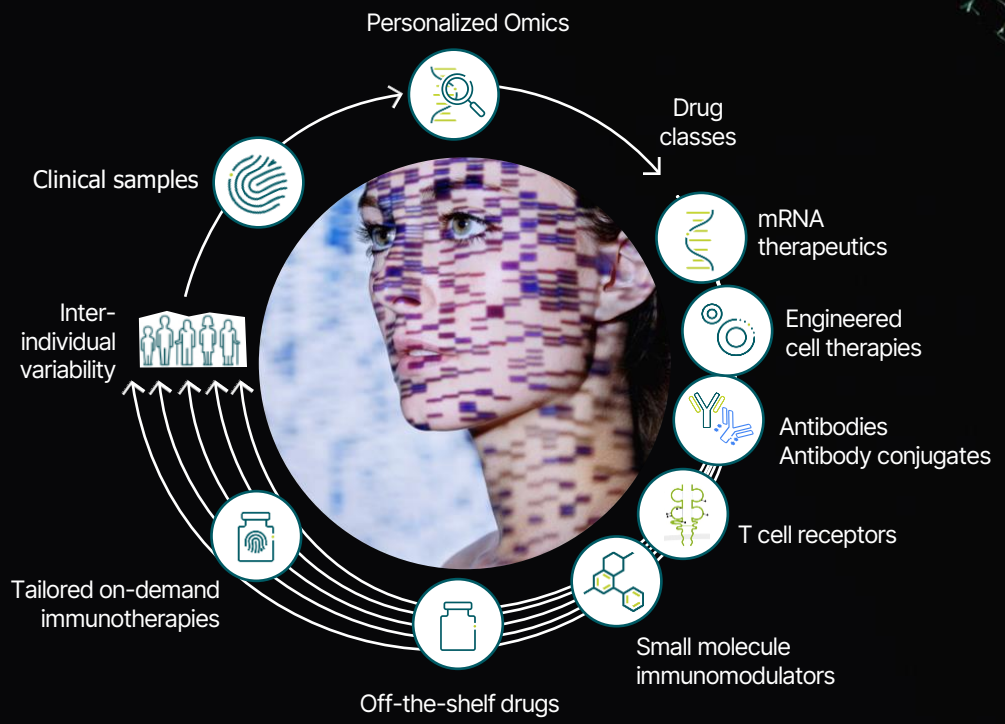
mRNA cancer vaccines

- Could eliminate polyclonal residual disease with individualized vaccines for potential long-term impact
- Polyspecific activity by targeting multiple antigens at once

ADC = antibody-drug conjugate; CAR = chimeric antigen receptor; TCR-T = T-cell receptor engineered T cell; IO = immune oncology.

Charting the Course for Tomorrow's Personalized Medicine

- Deep genomics & immunology expertise to analyse patient data
- Individualized treatment platforms to address inter-individual variability
- AI & digitally-integrated target & drug discovery and development
- In-house manufacturing



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BioNTech and InstaDeep – The Road to Partnership

2011
BioNTech introduces computationally designed individualized mRNA cancer vaccines[1]

2014
BioNTech initiates individualized mRNA cancer vaccine first-in-human trial[2]

2017
BioNTech rolls out an in silico neo-antigen selection process[3]

2019
BioNTech and InstaDeep begin project work

2020
BioNTech and InstaDeep create joint AI Lab with committed budget and dedicated infrastructure

2022
BioNTech invests in InstaDeep Series B round alongside Google and syndicate of investors

2022
BioNTech and InstaDeep work hand-in-hand to embed AI across BioNTech platforms and functions

2023
BioNTech acquires InstaDeep to operate as a wholly owned AI subsidiary

1. Cancer Res., PMID 22237626, 2. Nature PMID 25901682, Nature PMID 28678784, 3. BioNTech's personalized cancer vaccine candidate, autogene cevumeran, is partnered with Genentech, a member of Roche Group.

Two Companies: One Mission

BioNTech: >6,800[1] Employees	HQ: Mainz, Germany	Developing medicines to fight cancer, infectious diseases and other serious diseases.
InstaDeep: >370[1] Employees	HQ: London, UK	Focused on productizing disruptive AI innovation

Our Goal: Building a leading AI-first, personalized immunotherapy platform

(and leveraging the breakthroughs obtained in the process)

1. As of 30 June 2024

Our Goal: Deploying AI end-to-end in our immunotherapy pipeline

AI-first Immunotherapy Platform

1. Immunohistochemistry → 2. DNA/RNA sequencing → 3. Proteomics → 4. Protein Design → 5. Lab Functional Validation

Histology

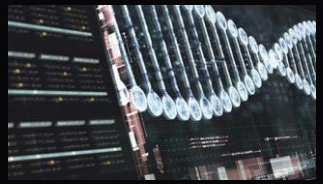
AI computer vision to improve speed and accuracy of tissue labeling

AI Vision

DNA

Sequence analysis and personalized genomic annotations

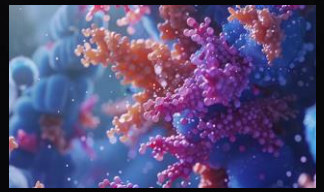
DNA LLMs



Proteomics

Leveraging AI for target discovery and analysis of the immunological landscape

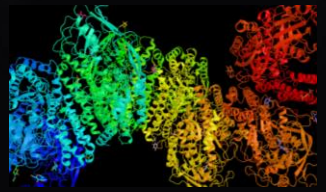
Protein LLMs



Protein Design

Developing assets for immunotherapy modalities (antibodies, cytokines, TCRs)

Protein LLMs



Lab

Instrument automation and quality control

AI Agent

Our Approach:

1. Scaling AI capabilities
2. Deploying across the pipeline

Part I.

Scaling AI Capabilities

Computing Infrastructure

InstaDeep's Supercomputing Cluster

Cluster Specifications
224 Nvidia H100 GPUs
86,000 CPU Cores
1.7 PetaBytes persistent storage
400 Gbps RoCE network

Source: Internal Data

Our Supercomputing Cluster Is Nearing Exascale Levels:

InstaDeep on-premise Cluster totals to ~0.5 ExaFLOPS

Top 100 worldwide [1]

Top 20 H100 GPU clusters worldwide [2]

[1] "Top 500, The List", June 2023
[2] "State of AI Report Compute Index", August 2024

Advanced In-House Rack Design

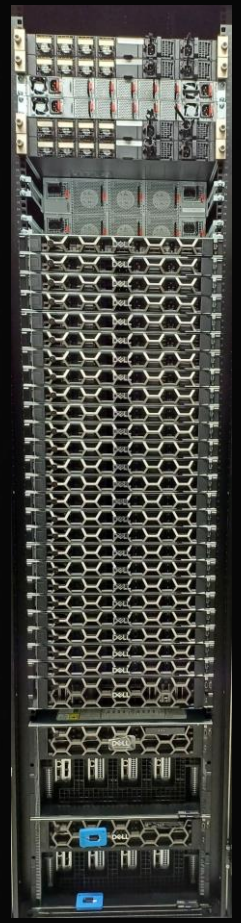
Easy to expand with modular nodes

Consistent performance, cost, power, cooling

Optimized for large-scale AI workloads

Simplified management with consistent architecture

Minimize expenses with standard design



Source: Internal Data

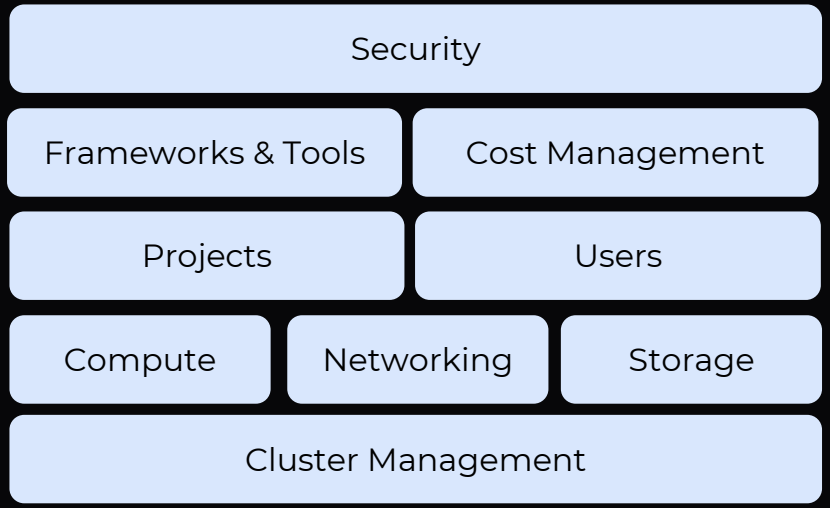
Software Stack Supporting our Cluster:

Alchor

Fully tailored AI stack from hardware to experiments

Open standards

Cutting-edge tooling



Strategic Benefits from our SuperComputing Cluster

- Availability when most needed
- Flexibility on Sw/Hw Integration
- No Vendor Locking
- Repeatable design
- Predictable costs
- Cost efficient (**50% savings** on cloud equivalent at 60% usage)

Scaling Intelligence

Scaling Intelligence

Why

Scaling Laws

How

Engineering Expertise

What

Accelerating Scientific Discovery

Scaling Intelligence

Why

Scaling Laws

How

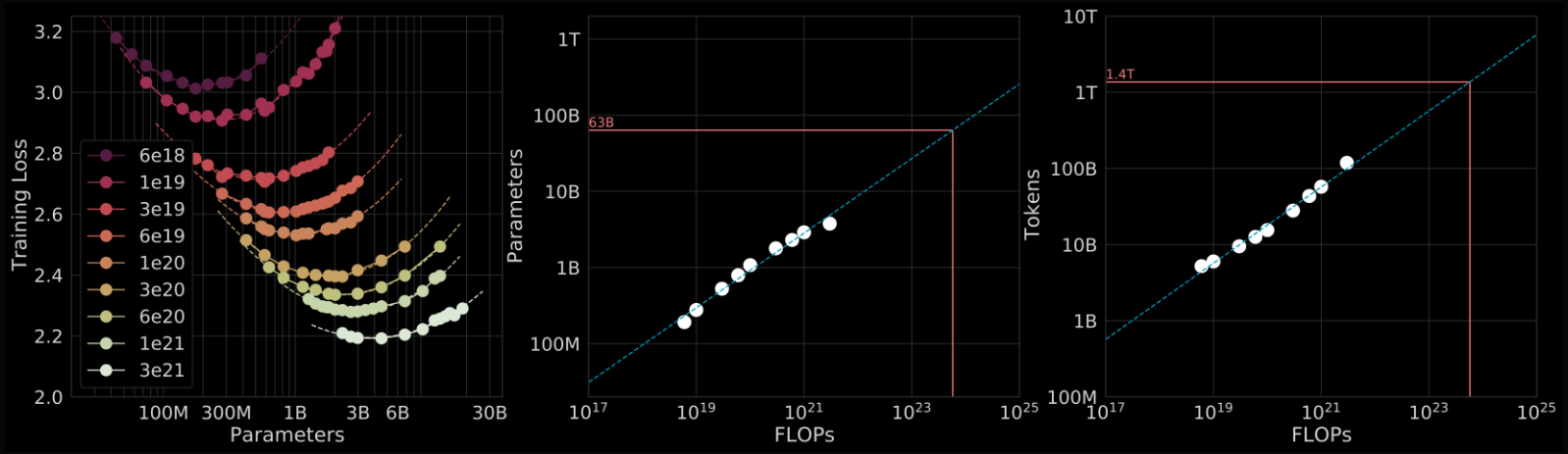
Engineering Expertise

What

Accelerating Scientific Discovery

Scaling Laws

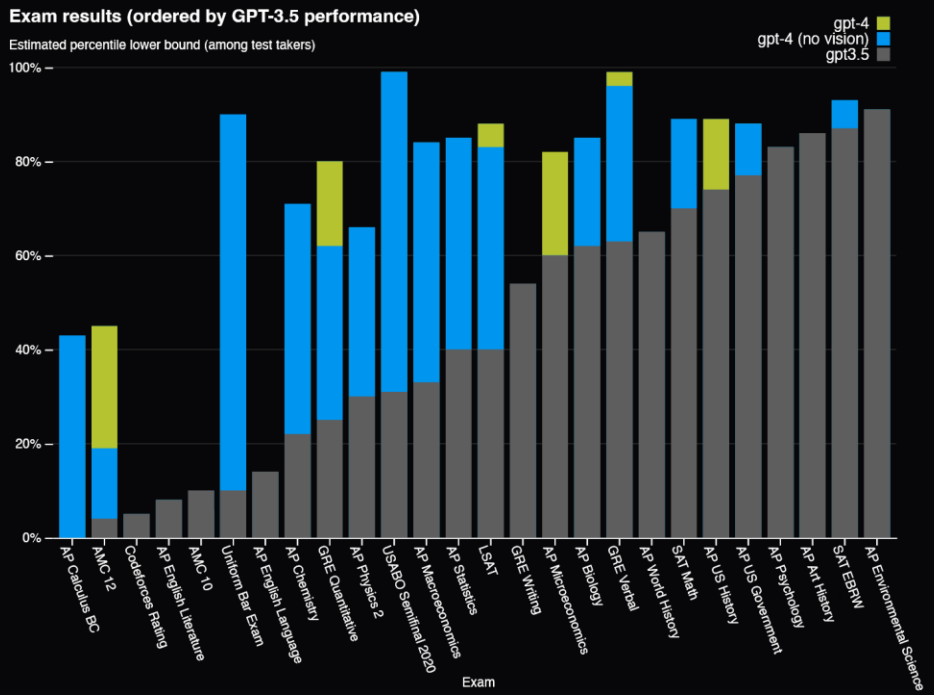
Performance of Large Language Models (LLMs) is a smooth, well-behaved and predictable function of the **number of parameters** of your model, the **amount of data** used to train it, and **computing resources**.



Source: Hoffmann, J., Borgeaud, S., Mensch, A., Buchatskaya, E., Cai, T., Rutherford, E., Casas, D.D.L., Hendricks, L.A., Welbl, J., Clark, A. and Hennigan, T., 2022. Training compute-optimal large language models.

Scaling Laws

We can expect **"more intelligence" by scaling** existing algorithms.



Source: Achiam, Josh, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida et al. "Gpt-4 technical report." (2023)

Scaling Intelligence

Why

Scaling Laws

How

Engineering Expertise

What

Accelerating Scientific Discovery

How to Scale Next-Generation Foundation Models

Scaling next-generation AI systems demands advanced engineering solutions, tightly with the hardware to balance training and deployment constraints.

Memory

Model Sharding
Rematerialization
Quantization / Precision

Network

Compute/Comm. overlap
I/O and Data processing
Hardware and Topology

Compute

XLA optimization
Kernel Fusion and Caching
Data Parallelism

Scaling Intelligence

Why

Scaling Laws

How

Engineering Expertise

What

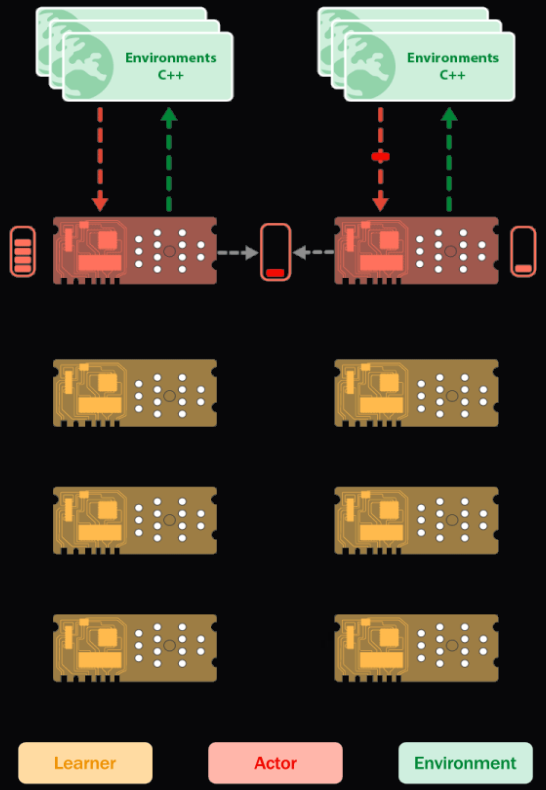
Accelerating Scientific Discovery

#1 Accelerating Reinforcement Learning

Reinforcement Learning is the science of **learning from trials and errors.**
A simulation engine **turns computation into data.**

Scaling Reinforcement Learning

- Multiple threads keep the **hardware accelerators** active.
- Learner cores process experience, synchronizing updates using **JAX primitives**.
- The architecture can be **replicated across a large number of nodes** to form a supercomputing cluster.
- Leverage **the high-speed inter chip interconnects** between the nodes of the hardware accelerators.

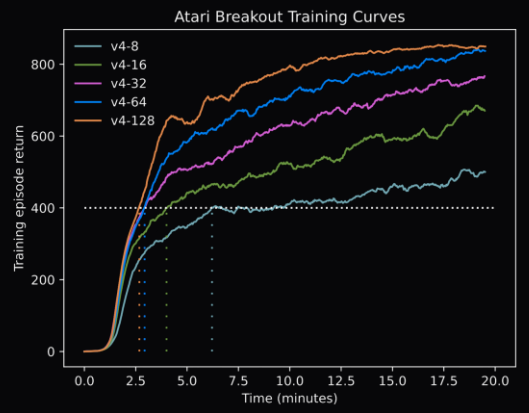


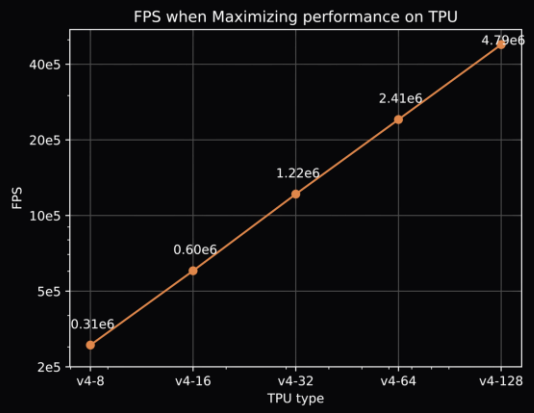
The Sebulba Architecture on 8x hardware accelerators[1]

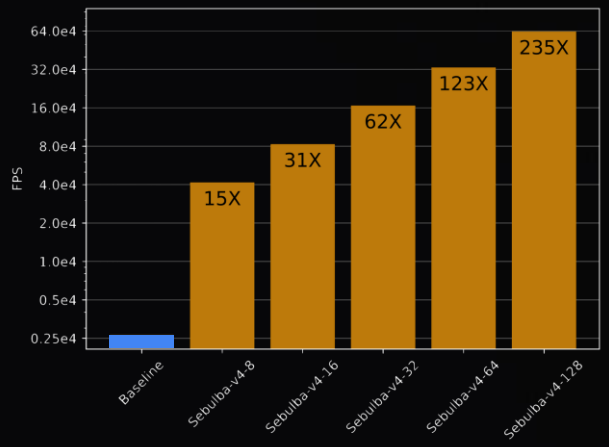
[1] "InstaDeep's scalable reinforcement learning on Cloud TPU", October 19, 2023, Google Cloud blog post
[2] Berner, C., Brockman, G., Chan, B., Cheung, V., Dębiak, P., Dennison, C., Farhi, D., Fischer, Q., Hashme, S., Hesse, C. and Józefowicz, R., 2019. Dota 2 with large scale deep reinforcement learning.
[3] Hessel, M., Kroiss, M., Clark, A., Kemaev, I., Quan, J., Keck, T., Viola, F. and van Hasselt, H., 2021. Podracer architectures for scalable reinforcement learning.

#1 Accelerating Reinforcement Learning

Better: 50% improvement in performance as we scale the hardware and simulated data.
Cheaper: 13x cost reduction due to the more efficient use of the hardware.
Faster: 240x faster to train an RL agent up to convergence.







[1] "InstaDeep's scalable reinforcement learning on Cloud TPU", October 19, 2023, Google Cloud blog post
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[3] Hessel, M., Kroiss, M., Clark, A., Kemaev, I., Quan, J., Keck, T., Viola, F. and van Hasselt, H., 2021. Podracer architectures for scalable reinforcement learning.

#2 Generative AI for Biology

Scaling the Next-Generation of our Generative AI Models

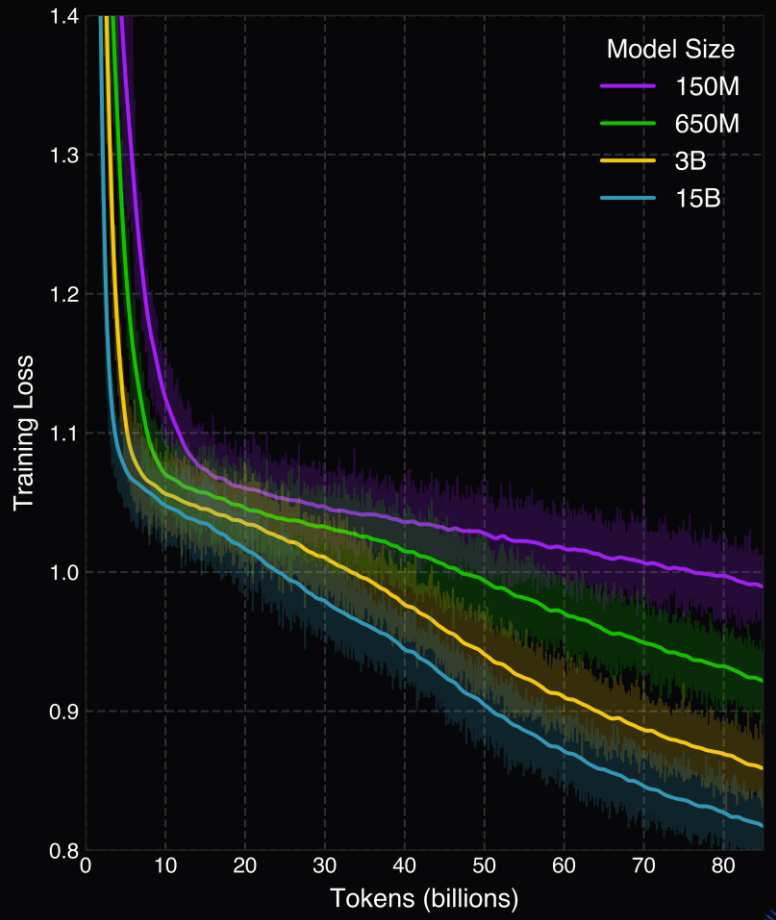
- in-house JAX-based software library
- best-in-class engineering for scaling LLMs

  e.g. Hybrid Parallelism, mixed-precision, rematerialization, etc.

Results

- Train multi-billion parameters models (+15B)
- Scaling Laws in Action
- Hardware efficiency on par with the latest Meta Llama 3.1[1]

  i.e. Model Flop Utilization of ~50% for our 15B model



Source: InstaDeep

[1] Dubey, A., Jauhri, A., Pandey, A., Kadian, A., Al-Dahle, A., Letman, A., Mathur, A., Schelten, A., Yang, A., Fan, A. and Goyal, A., 2024. The llama 3 herd of models. *arXiv preprint arXiv:2407.21783.*

Summary

InstaDeep's Supercomputing Cluster and advanced software stack could facilitate new scientific breakthroughs, services and products that were previously out of reach.

Scaling Laws

Engineering Expertise

Accelerating Scientific Discoveries

AI Innovation

Bayesian Flow Networks

Generative AI

Sora: generative AI model for videos

OpenAI 2024

A stylish woman walks down a Tokyo street filled with warm glowing neon and animated city signage...

Source: SORA blog post by OpenAI: https://openai.com/index/sora/

Joint Probability Distributions

For a generative model of face images, creating a new face means picking a sample from the joint probability distribution of all the pixels.

Q: Why is this so hard?

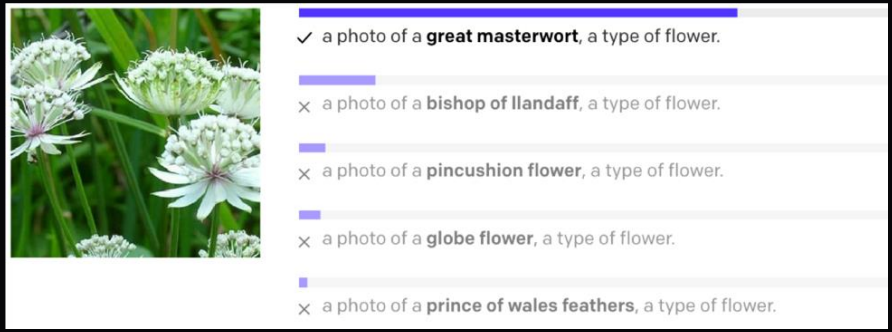
A: Because all the pixels are interrelated

Generating Diverse High-Fidelity Images with **VQ-VAE-2** (Razavi et al. 2019)

Steerable Generation

We want to control what we generate.

With a multimodal model (e.g. images and text) we can do this with conditional sampling: fix one modality, generate another.



Given an image, generate a caption (**CLIP** OpenAI 2021)

Given an prompt, generate an image (**DALL·E** OpenAI 2021)

One Model, Many Tasks

Learning a joint distribution over many variables then choosing which to fix and which to generate gives us one model for many tasks

But which Model?

Diffusion

Pros: Continuous data (especially images), inpainting, fast gradient-based sampling

Cons: Discrete data

Autoregression (GPT)

```
                                slides
Sorry boss the dog ate my ______
```

Pros: Sequence data (especially text)

Cons: Unordered data, inpainting, slow sampling

Masked prediction (BERT)

```
      boss     cat        report
Sorry ____ the ___ ate my ______
```

Pros: Discrete data, inpainting, representation learning

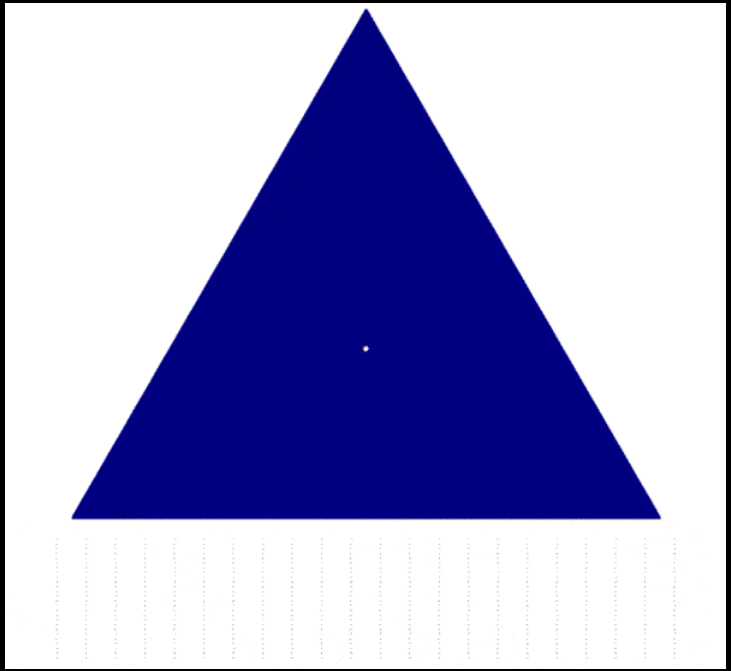
Cons: Continuous data, slow sampling

Bayesian Flow Networks

BFNs are a new class of generative model that uses Bayesian inference to update beliefs about data.

Unlike diffusion models, they generate discrete data in a continuous way, allowing for gradient-based sampling

This makes BFNs well-suited for controllable generation across diverse data modalities.



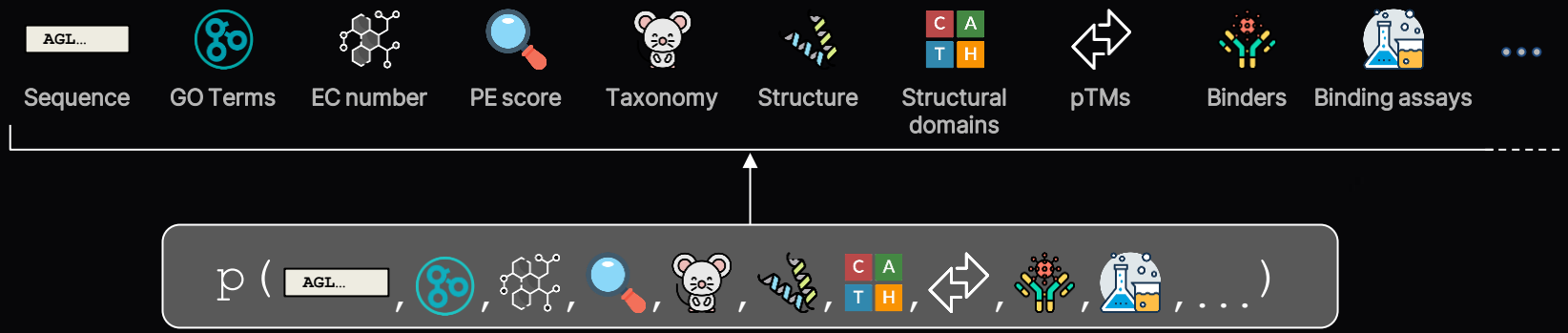
Graves, Srivastava, Atkinson, Gomez 2023

Generative Modelling

A unifying framework to learn useful functions from data

(1) Learn to **model the joint distribution of *all* your data**, and (2) **conditionally sample for tasks of interest.**

Proteomics: Joint Modelling

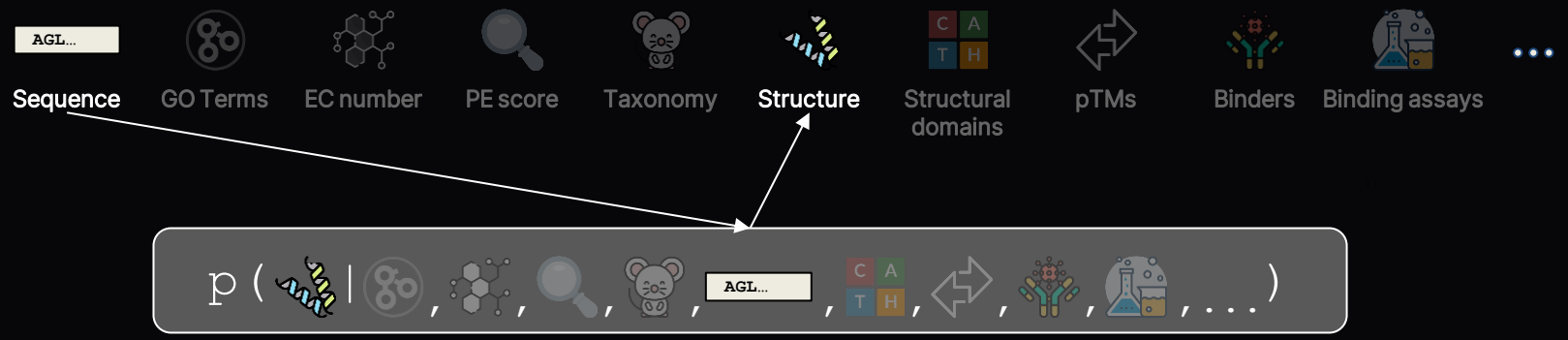


Generative Modelling

A unifying framework to learn useful functions from data

(1) Learn to **model the joint distribution of *all* your data**, and (2) **conditionally sample for tasks of interest.**

Proteomics: Protein Folding



Generative Modelling

A unifying framework to learn useful functions from data

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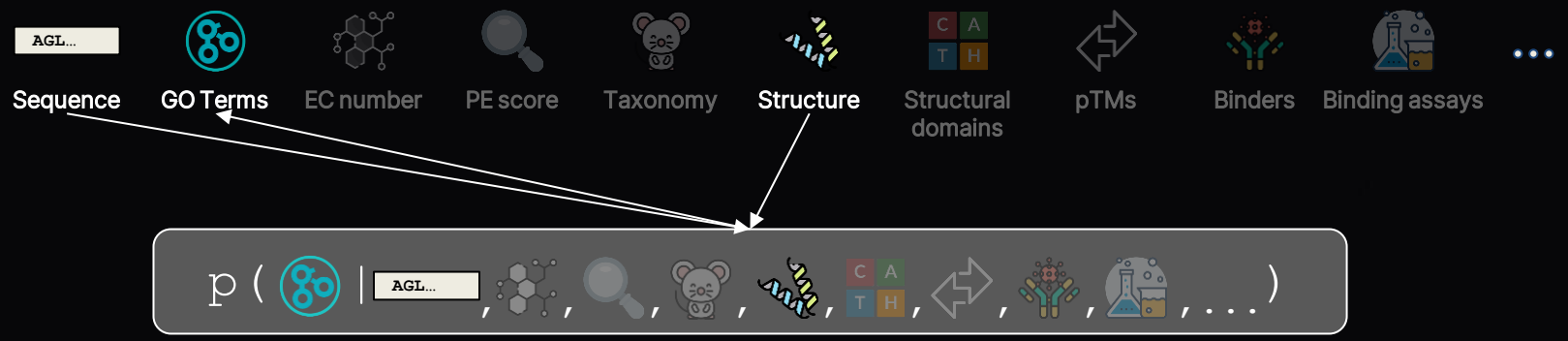
Proteomics: Function Prediction

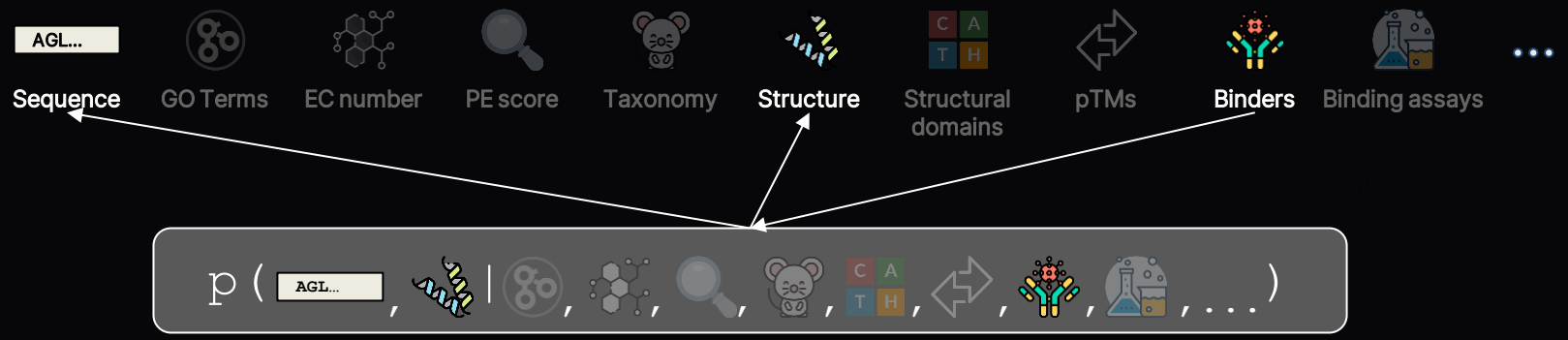


Generative Modelling

A unifying framework to learn useful functions from data

(1) Learn to **model the joint distribution of *all* your data**, and (2) **conditionally sample for tasks of interest.**

Proteomics: Antibody Design



Generative Modelling

A **unifying framework** to learn useful functions from data

(1) Learn to **model the joint distribution of *all* your data**, and (2) **conditionally sample for tasks of interest.**

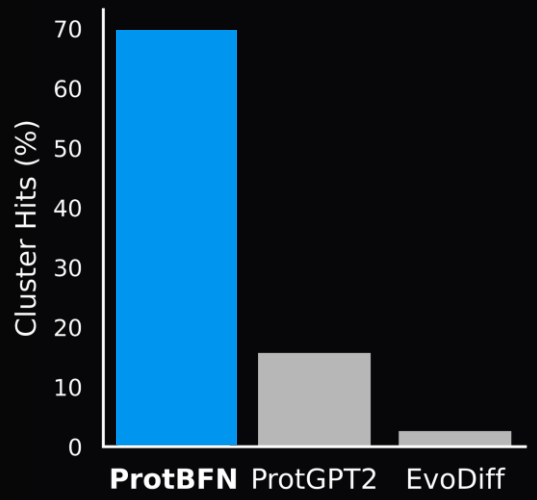
Proteomics: Sequence Generation

			De Novo	Conditional
AGL... Sequence	Autoregression (GPT) →	R MPPR____...	*Yes*	*Limited*
	Masked prediction (BERT) →	RRS MPP___IV...	*No*	*Yes*
	"Discrete" diffusion →	P R I MMPRSSPV...	*Limited applicability to discrete data*	

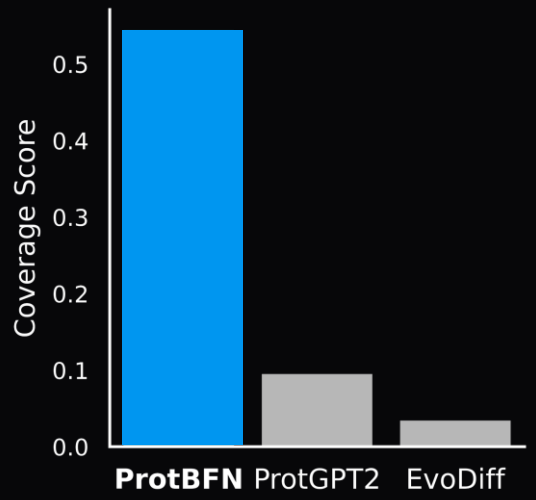
Natural, Diverse & Novel Protein Sequences

ProtBFN learns statistical and biochemical properties of natural proteins with high-fidelity.

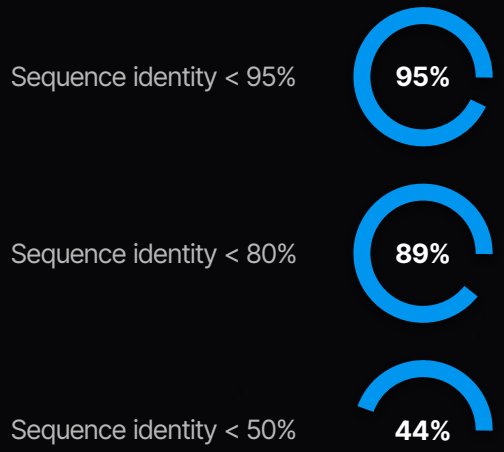
More natural...[1]



...more diverse...[1]



...and highly novel.[2]



1. 10,000 generated sequences from each model are matched to clusterings from UniRef50. A hit is determined as a match with >50% sequence identity. Coverage score is the ratio of the number of unique clusters hit to the expected number if sequences were drawn i.i.d. from the models training distribution. ProtGPT2 (huggingface.co/nferruz/ProtGPT2) and EvoDiff (github.com/microsoft/evodiff) sequences are sampled using publicly available code and model weights provided by the authors.
2. Identity of ProtBFN generated sequences to the best matching protein sequence found in the models training data. Any identity < 100% is a novel sequence that the model has not seen before.

Globular Structural Motifs With Novel Sequences

Predicted structures of generated sequences show natural, globally coherent and functionally diverse folds.

Structure largely determines function in nature.

Single and multi-domain proteins.

Globally coherent generations with inter-domain interactions.

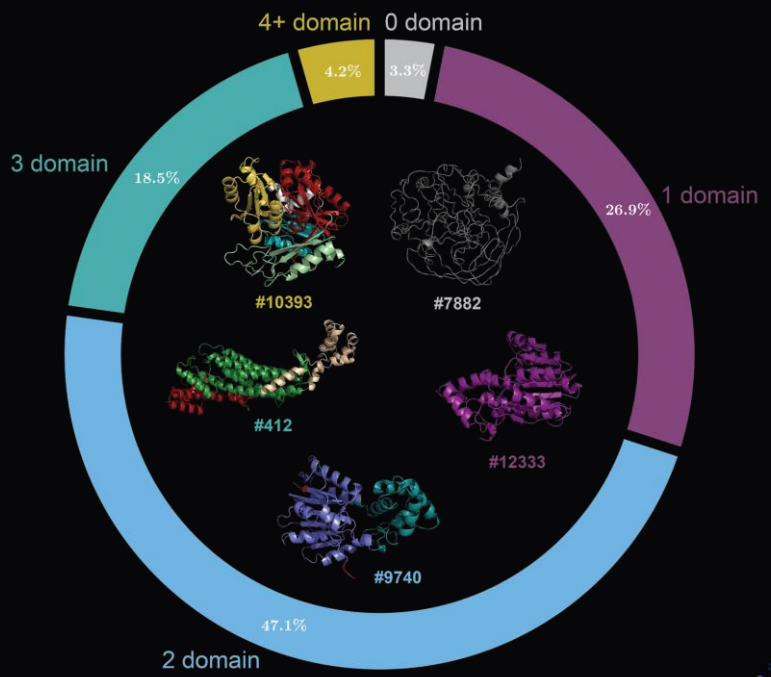
Spans diversity of known structures and tree-of-life.

Alpha Helical, Beta Sheet, Alpha-Beta and Irregular domains.

Small and large domains.

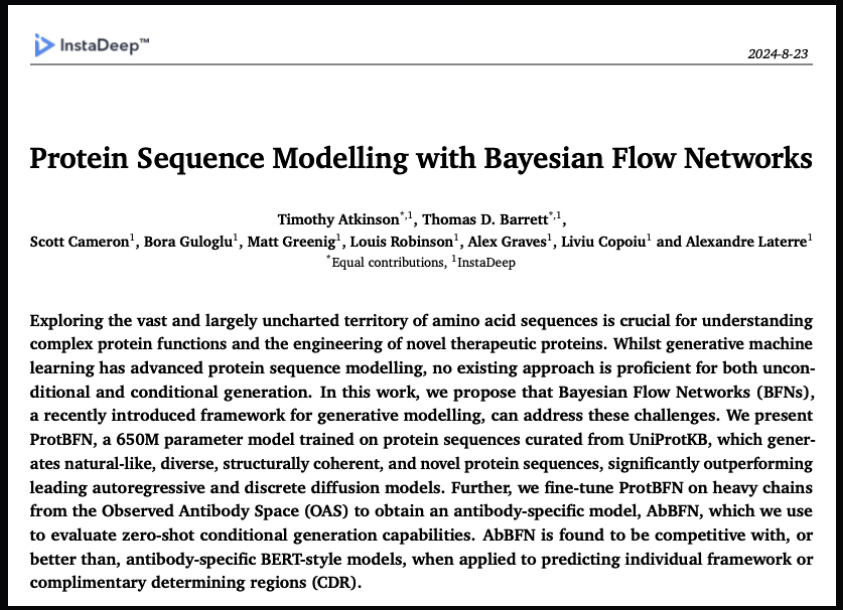
Transmembrane Proteins (porins and transporters) and Enzymes.

Domains specific to Archaea, Bacteria, Eukarya (Plants, Humans).



BFN for Protein Sequences

- Outperforms or matches task-specific autoregressive, diffusion and BERT models.
- Improved naturalness, diversity and novelty.
- Uses zero-shot conditioning of model.
- Patent application filed.



InstaDeep™ 2024-8-23

Protein Sequence Modelling with Bayesian Flow Networks

Timothy Atkinson[*,1], Thomas D. Barrett[*,1],
Scott Cameron[1], Bora Guloglu[1], Matt Greenig[1], Louis Robinson[1], Alex Graves[1], Liviu Copoiu[1] and Alexandre Laterre[1]
[*]Equal contributions, [1]InstaDeep

Exploring the vast and largely uncharted territory of amino acid sequences is crucial for understanding complex protein functions and the engineering of novel therapeutic proteins. Whilst generative machine learning has advanced protein sequence modelling, no existing approach is proficient for both unconditional and conditional generation. In this work, we propose that Bayesian Flow Networks (BFNs), a recently introduced framework for generative modelling, can address these challenges. We present ProtBFN, a 650M parameter model trained on protein sequences curated from UniProtKB, which generates natural-like, diverse, structurally coherent, and novel protein sequences, significantly outperforming leading autoregressive and discrete diffusion models. Further, we fine-tune ProtBFN on heavy chains from the Observed Antibody Space (OAS) to obtain an antibody-specific model, AbBFN, which we use to evaluate zero-shot conditional generation capabilities. AbBFN is found to be competitive with, or better than, antibody-specific BERT-style models, when applied to predicting individual framework or complimentary determining regions (CDR).

Released only a few days ago![1]

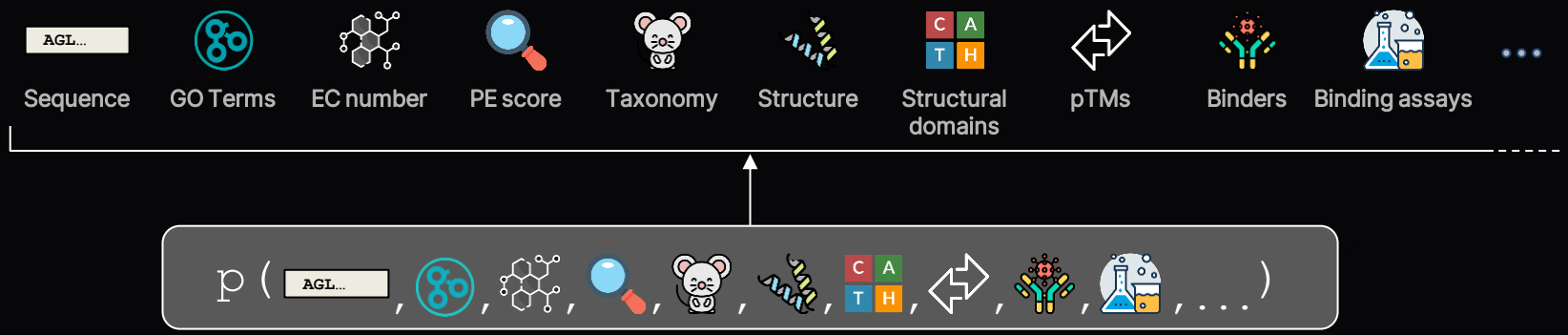
1. Available at https://www.biorxiv.org/content/10.1101/2024.09.24.614734v1

Going Beyond Sequence-Only Models

Our goal is to model everything: building foundational models of the joint distribution of heterogeneous scientific data.

Performance across multiple data types and sources.

Flexibility in the hands of scientists with task-specific inference.



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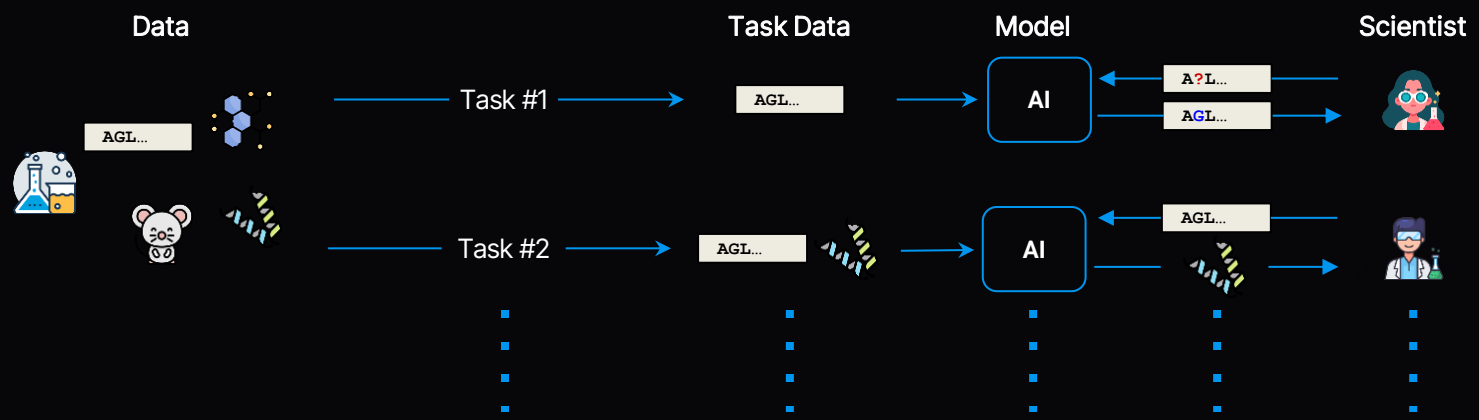
Conventional ML



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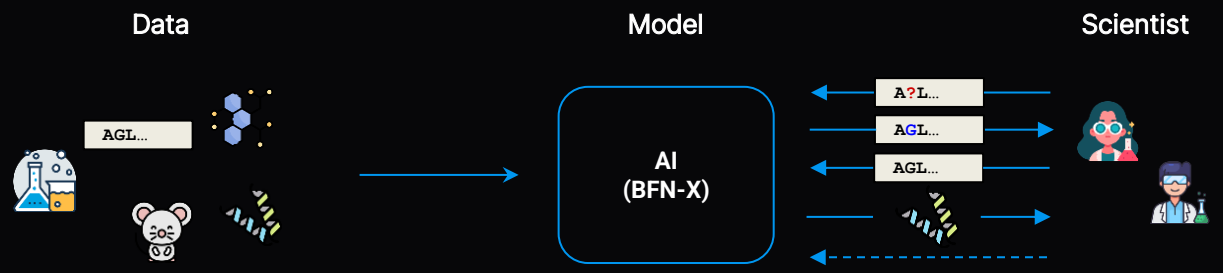
Our vision



Tasks determined flexibly at inference with conditional generation

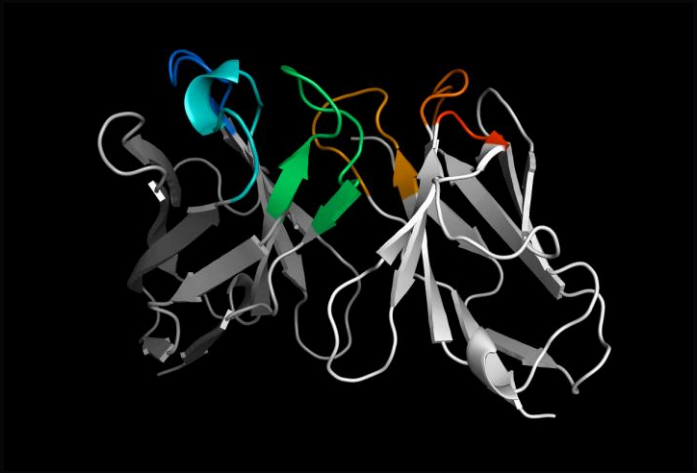
Introducing AbBFN-X

First look at our multimodal model for antibodies.

36 different attributes jointly modelled: sequence, genetic, biophysical

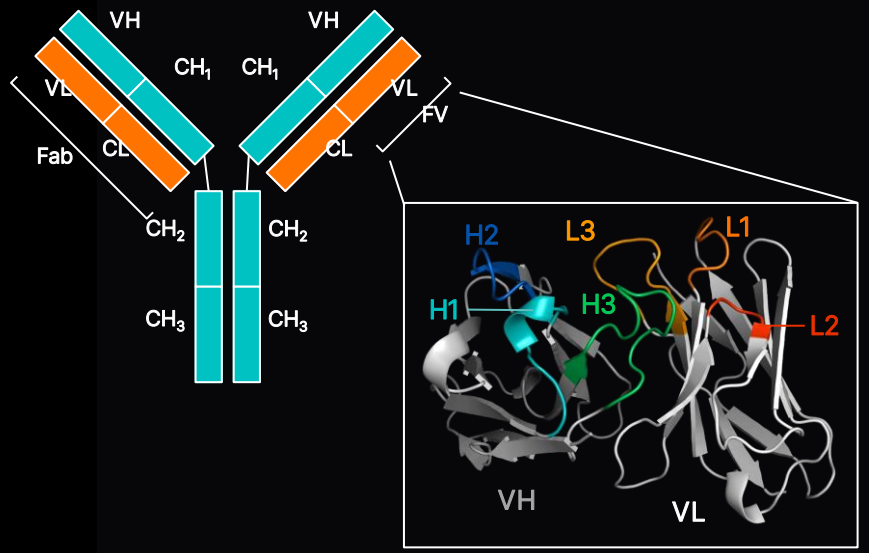
Empowers scientists with tunable generation, being highly flexible across many tasks.

Today's use cases go beyond standard AI-enhanced antibody design workflows.



Source: Generated Image

AbBFN-X



VH: EVQLLESGGGLVQPGGSLRLSCAAS**GFTFSSYA**MSWVRQAPGKGLEWVSA**ISWNSGSI**YADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYYC**ARGWSQVDTAMDLDY**GQGTLVTVSS

CDR-H1 *CDR-H2* *CDR-H3*

V gene *D gene* *J gene*

VL: DIQMTQSPSSVSASVGDRVTITCRAS**QSVSSN**LAWYQQKPGKAPKLLIY**GAS**SLQSGVPSRFSGSGSGTDFTLTISSLQPEDFATYYC**QQYNNWLT**FGQGTRLEIK

CDR-L1 *CDR-L2* *CDR-L3*

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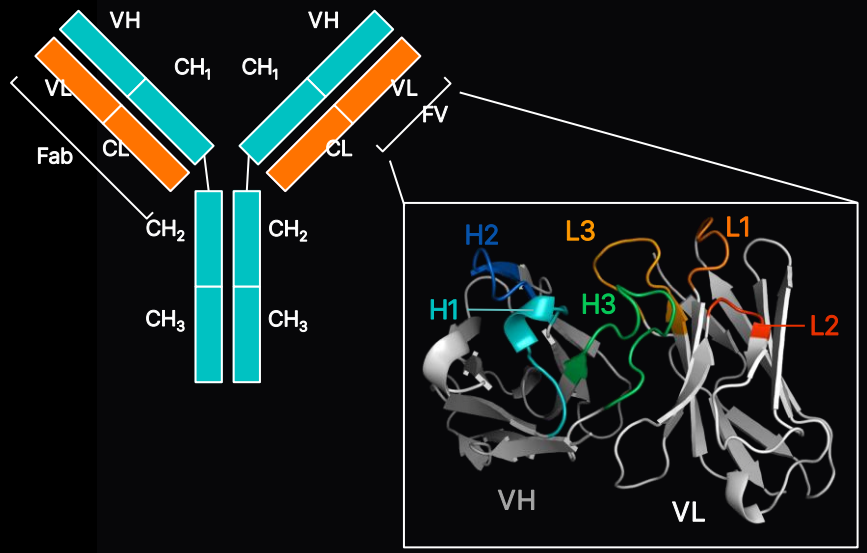
AbBFN-X



Amino acid sequence

- FWR-H1
- CDR-H1
- FWR-H2
- CDR-H2
- FWR-H3
- CDR-H3
- FWR-H4
- FWR-L1
- CDR-L1
- FWR-L2
- CDR-L2
- FWR-L3
- CDR-L3
- FWR-L4

Genetic Attributes

- HV gene
- HD gene
- HJ gene
- LV gene
- LD gene
- LC locus
- HV seq. identity
- HD seq. identity
- HJ seq. identity
- LV seq. identity
- LJ seq. identity
- Species

Biophysical Attributes

- Hydrophobicity
- Positive Patches
- Negative Patches
- Charge Imbalance

Length Attributes

- CDR-H1 length
- CDR-H2 length
- CDR-H3 length
- VH length
- CDR-L1 length
- CDR-L2 length
- CDR-L3 length
- VL length

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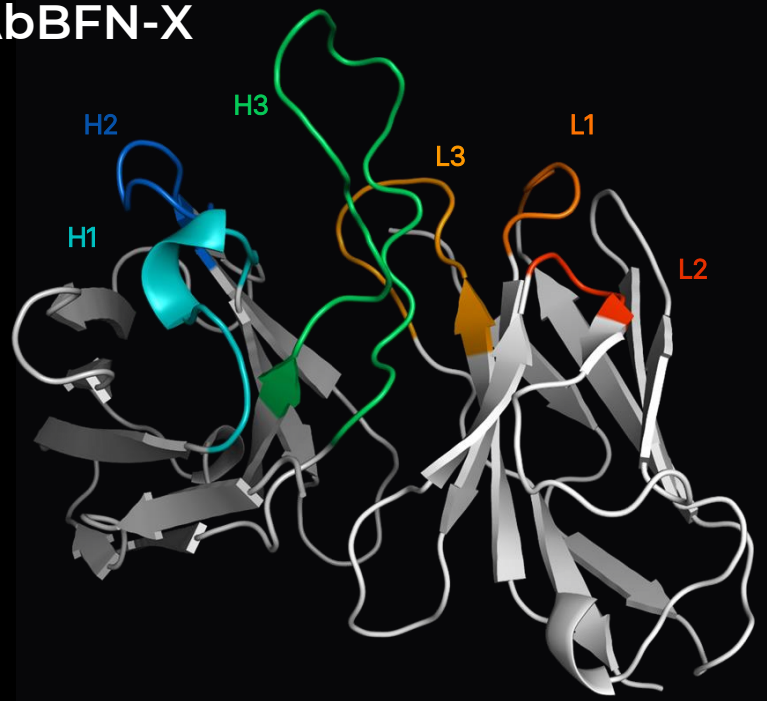

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- FWR-H4
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- CDR-L1
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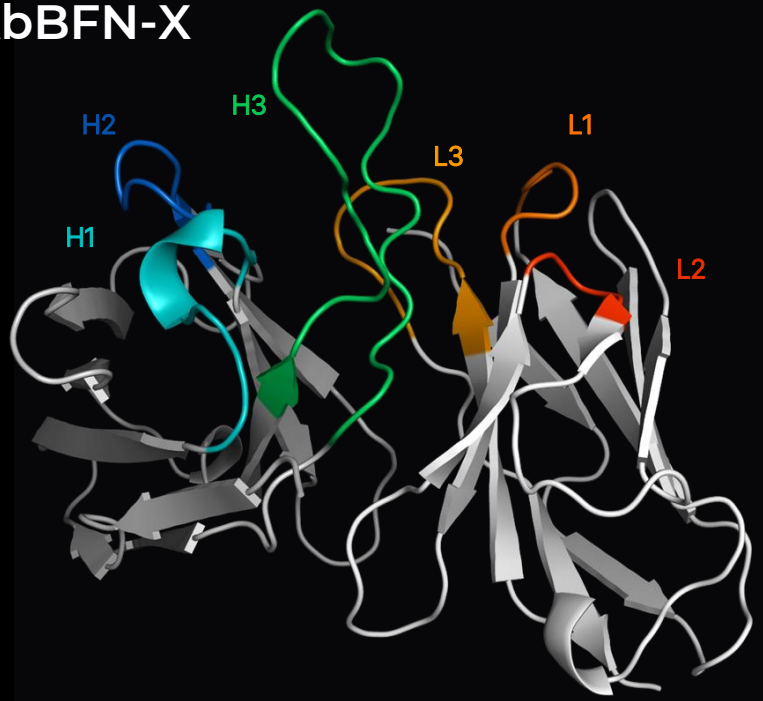
AbBFN-X



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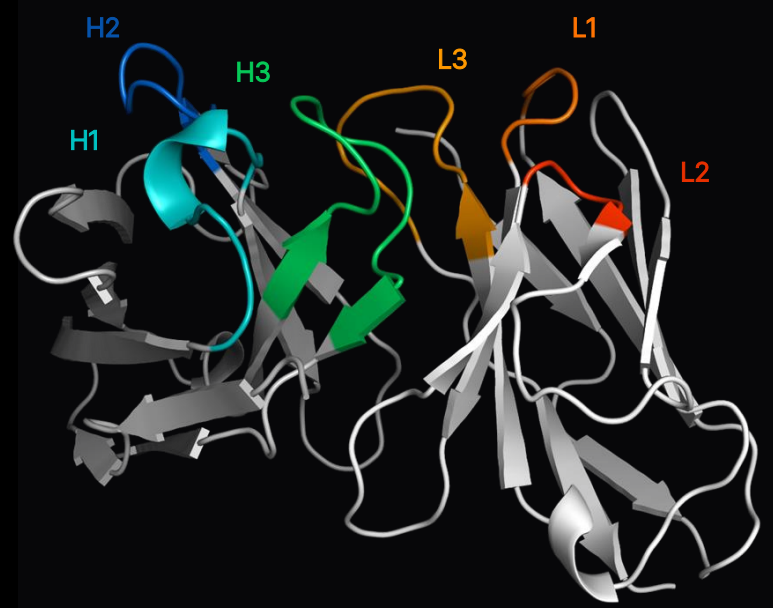
AbBFN-X



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Example Task 1: Anti-HIV Antibody Library Design

Generating a library of rare antibodies against HIV:

- Heavy chain synthesis. CDR-H3 design and grafting.
- Light chain library synthesis with desired CDR length.
- Paired library generation.
- Mutagenesis.
- Discard poor candidates.

Example Task 1: Anti-HIV Antibody Library Design

Generating a library of rare antibodies against HIV:
(1) identify target attributes.
(2) conditionally sample for rare, desired antibodies.

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CDR-H1	CDR-L1
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FWR-H3	FWR-L3
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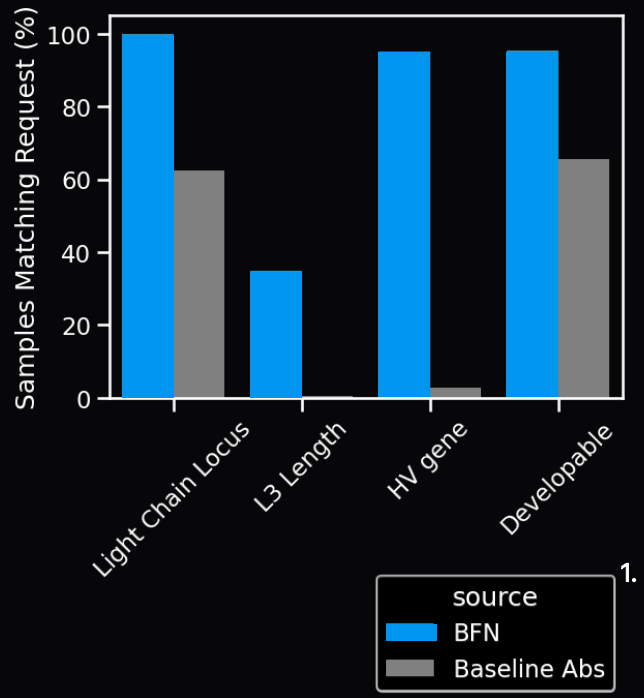

1.

AbBFN-X antibodies are 5600x more likely[2] to have all desired characteristics.

1. "Baseline Abs" refers to data sets of natural antibodies (Olsen *et al*, 2021, Prot. Sci.), "BFN" refers to samples generated by AbBFN-X.
2. compared to the rate of finding antibodies with the correct characteristics in data sets of natural antibodies (Olsen *et al*, 2021, Prot. Sci.)

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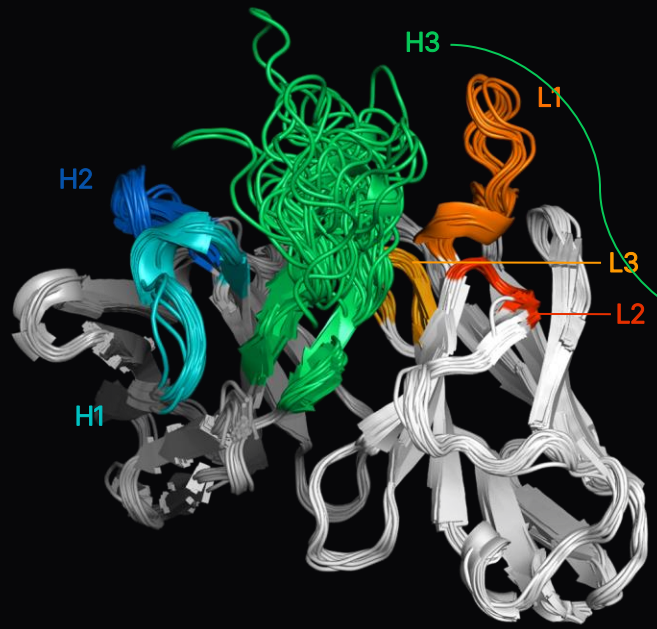


ARDEIYFLEWLISY
AKVRLGELPYEAFDI
ARGVRVQ SYNWFDP
ASGEYFFDTSSYPN
ARSSFVYPKSGYDFYFDY
ARDIAVDPESTAYFDY
AKGFSYGDGWADY
VRLRVGVLPGAFDI
ARDGGHYSH
ASGSGDSRYAQPLWFTTAFDI
ATSLNYGVIISD
ASGKMAVAYYFDY
AREGMDASMYYFDY
ARDMGYHDGALVFDN
⋮

Unique CDRs[1]	100%
Unique CDR-H3s	100%
Unique CDR-L3s	99%
Unique non H/L3 CDRs	52%

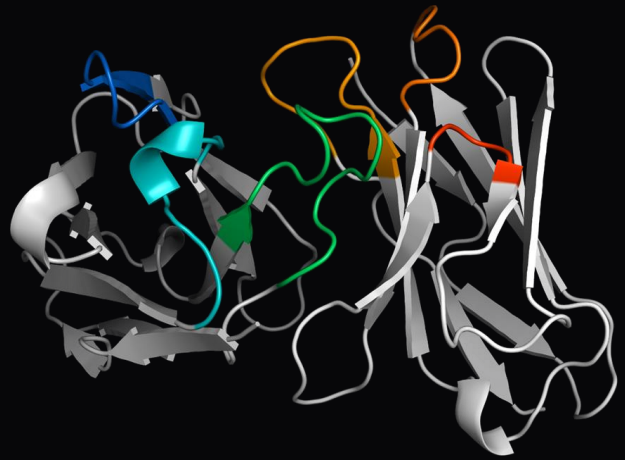
1. 128 samples were generated, uniqueness assessed by considering all relevant regions at once, excluding framework regions.

Example Task 2: Heavy-Light Pairing

Generating a set of **developable** light chains that will **pair** with a heavy chain:

(1) **Condition** on desired properties and heavy sequence.

(2) **Sample** for **stable**, **diverse** sequences.



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CDR-H3 length	CDR-L3 length
VH length	VL length

Biophysical Attributes

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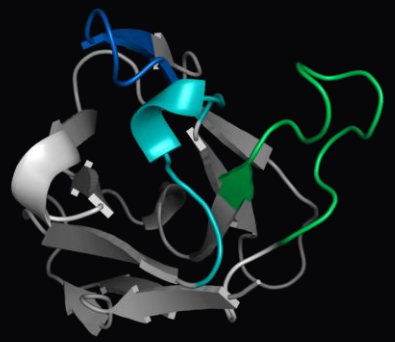

Conditioning on the required **heavy chain**

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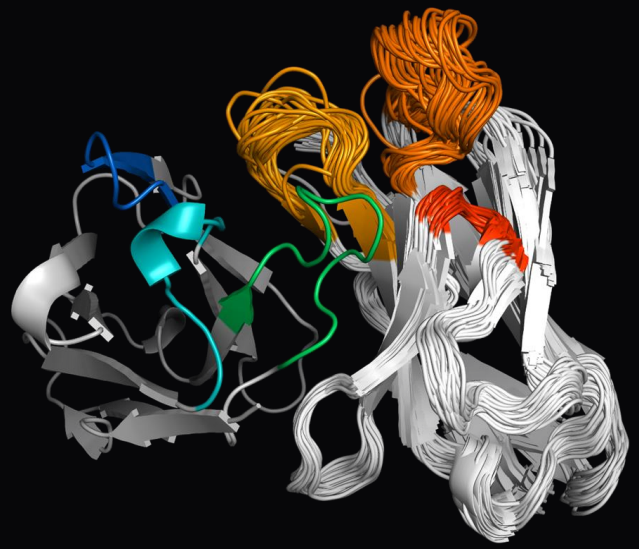

Conditioning on the required **heavy chain**

results in **diverse light chains** in length and structure

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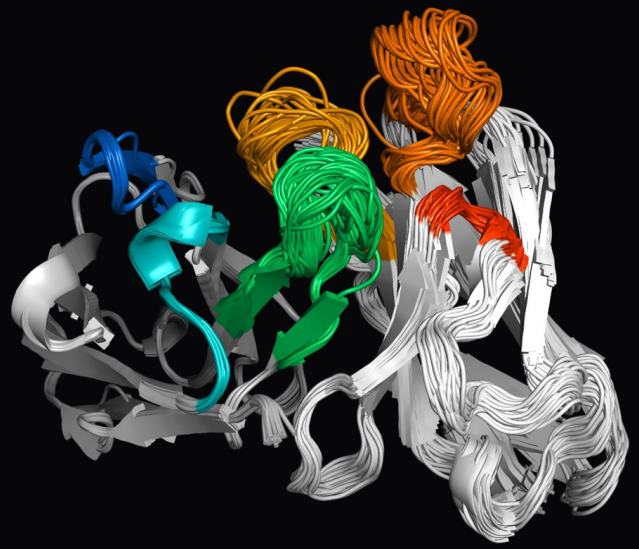


Conditioning on the required **heavy chain**

results in **diverse light chains** in length and structure

while respecting the **requested sequence** and generating **stable pairs**.

Generative AI for Proteomics

InstaDeep is developing **next-generation GenAI models** across the whole stack, from **fundamental ML research**, to modelling scientific data and **enabling new capabilities** for scientists.

Bayesian Flow Networks

Unified modelling of multi-modal data

- **All modalities** as first class citizens
- Joint learning of **heterogeneous data**
- Task-specific **conditional generation**

Protein Sequence Modelling

Published demonstrations

- **Leading performance** across tasks
- Diverse & novel ***de novo* generation**
- **Zero-shot** inpainting at inference

BFN-X

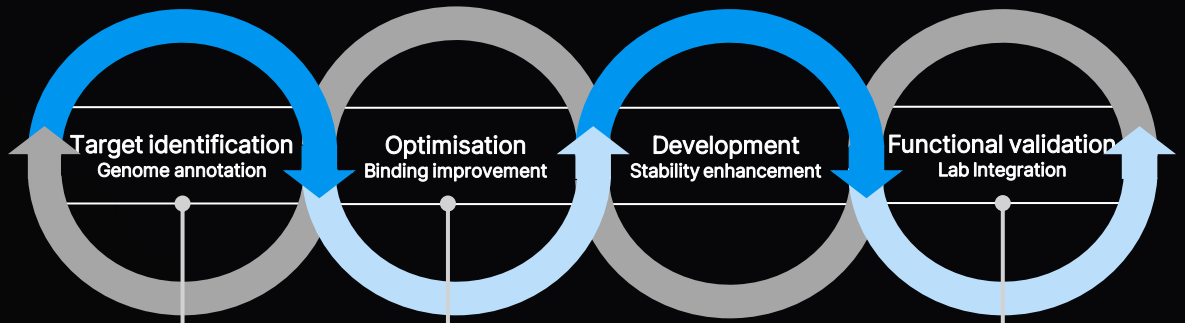
In-development foundation models

- **Sequence**, **genetic** and **biophysical**
- Learns **rational antibody principles**
- Enables **diverse suite of tasks**

DeepChain

One platform, Multiple tools

By combining State-of-the-art Science with Engineering, Our AI Tools aim to Accelerate the R&D pipeline



Nucleotide Transformers[2,3]

- Splicing prediction
- In silico design of regulatory sequences

Bayesian Flow Networks[1]

- De novo antibody design
- Affinity enhancement

Assistants

- Form hypotheses, design experiments - Call tools to analyse results collaborating with a human scientist

[1] Alice Sends Amino Acids to Bob: Protein Sequence Modelling with Bayesian Flow Networks, Barrett et al., Under Review (2024).
[2] The Nucleotide Transformer: Building and Evaluating Robust Foundation Models for Human Genomics, Dalla-Torre et al., Under Review (2023).
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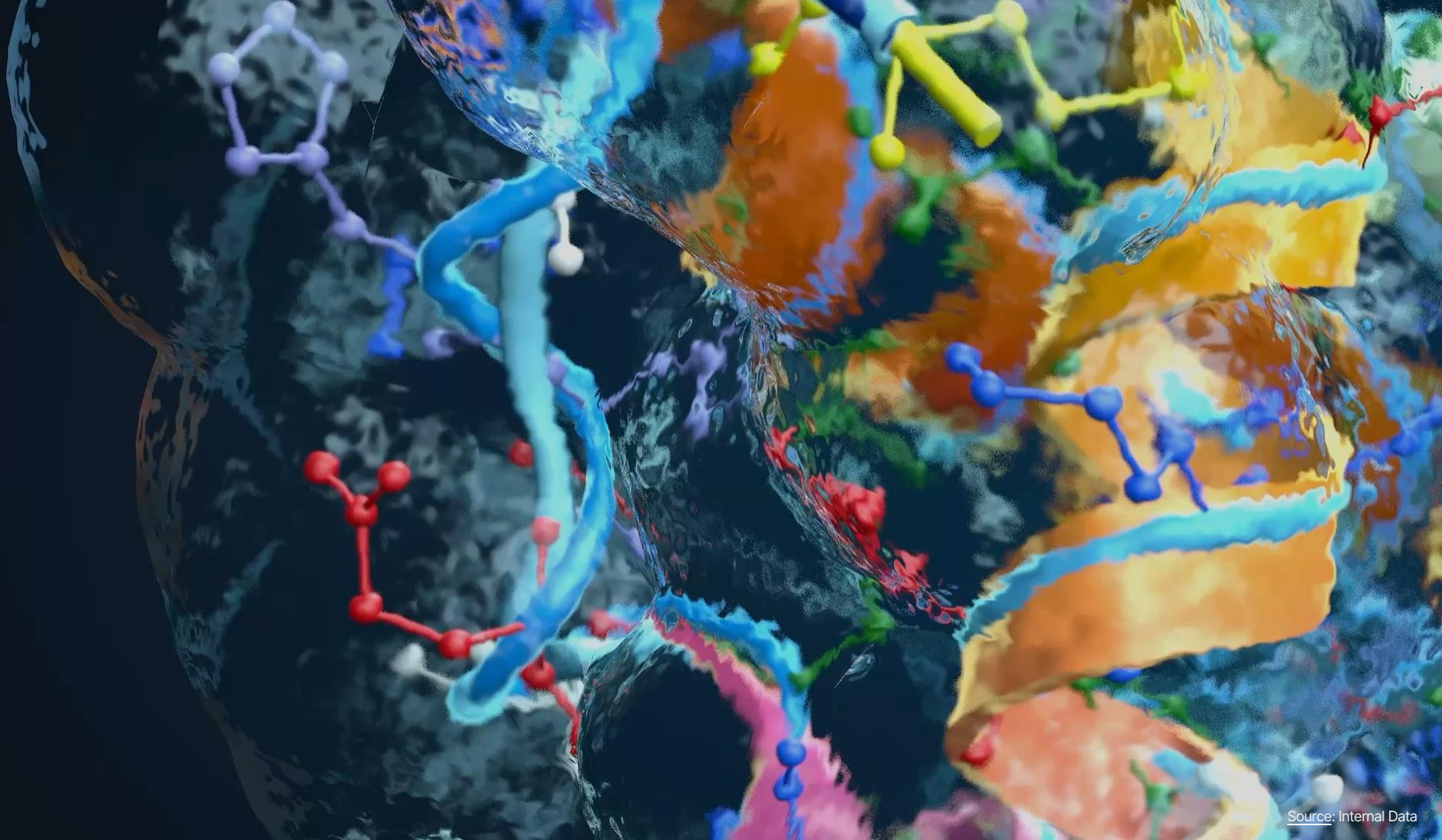

Source: Internal Data

We Are Releasing our Flagship Models on DeepChain

ProtBFN & AbBFN[1]

State-of-the-art generative protein models

✓ Generates natural-like, diverse, structurally coherent, and novel protein sequences

✓ Outperforms leading autoregressive and discrete diffusion models

✓ Enables flexible conditional generation in a zero-shot manner

Nucleotide Transformer[2] & SegmentNT[3]

Our foundation models for DNA

✓ Single nucleotide resolution

✓ Up to 50kb context length without performance drop

✓ Generalizes across species

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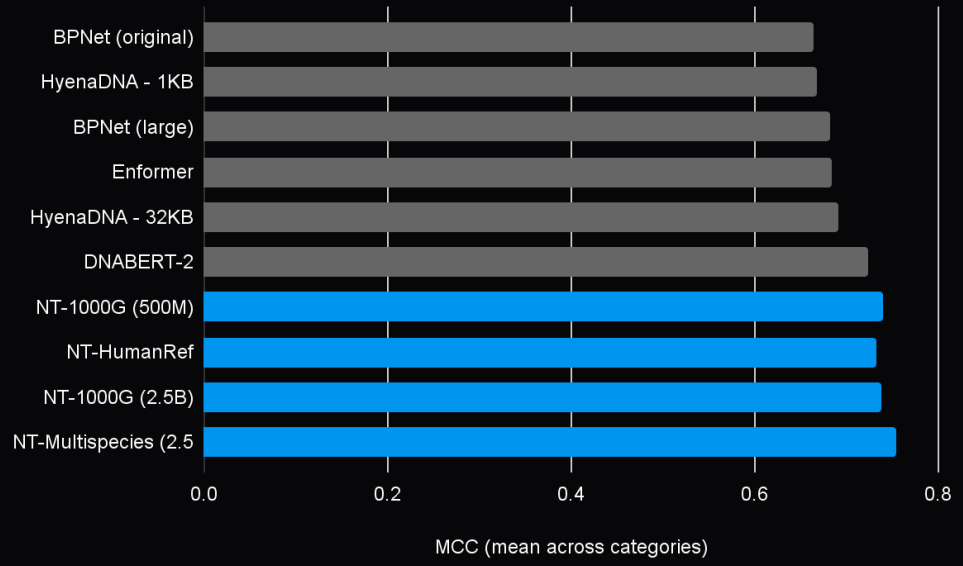
Our Foundation Models for Genomics are State-of-the-Art

Nucleotide transformer models are state-of-the-art in the space[1]



[1] The Nucleotide Transformer: Building and Evaluating Robust Foundation Models for Human Genomics, Dalla-Torre et al., Nat. methods (press)

+700K Downloads

Across model sizes[1]

One of the Most Downloaded Genomics AI Models on Hugging Face[2]

[1] Cumulative Downloads for Nucleotide Transformer models, 50-2.5B parameter sizes, September 2024. Hugging Face Statistics. Models Release Date: April 2023.
[2] Count by family of models under the "Genomics" official Hugging Face tag: https://huggingface.co/models?other=genomics&sort=downloads, September 2024.

We are releasing capabilities to build and scale with our AI models

01

Optimized Setup

02

03

01

Optimized Setup

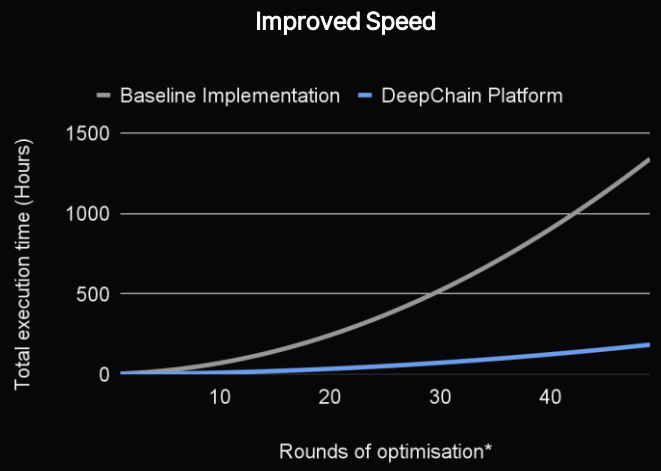
02

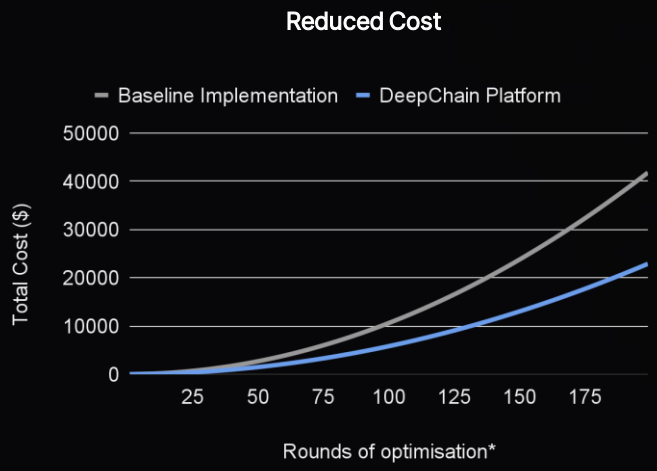
03

Get access to our hardware-accelerated workflows to run models with a few lines of code

Send a request to the Inference API and receive a fast response containing the model's output

Running inference with DeepChain is 7X faster and 2X cheaper for *in silico* design of regulatory sequences*





* reference methodology: Jores, T., Tonnies, J., Wrightsman, T. et al. Synthetic promoter designs enabled by a comprehensive analysis of plant core promoters. Nat. Plants 7, 842–855 (2021).
* Test implementation: Sequence length: 6kbp and 2.1kbp sequences, Parameters: --num_indels=8000, --prop_indels=0.5, --random_indels=True, --min_indels_size=2, --max_indel_size=5, --tissue_optimize_idx=1, --opt_metric=increase, --num_rounds=30
* Baseline implementation set-up: 1 NVIDIA V100 Tensor Core GPUs, using published Pytorch implementation available on Hugging Face

01

Optimized Setup

02

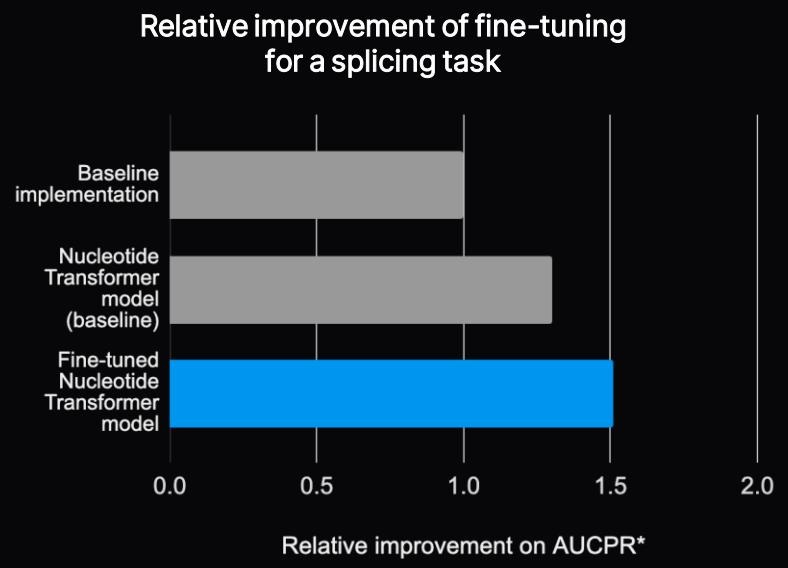
Customization

Customize models for your needs

Customize a model for a specific task via supervised fine-tuning with our proprietary parameter efficient fine-tuning methods

03

Fine-tuning a model on a specialised data set increased performance ≈1.5X for a splicing prediction use-case



* AUCPR: metric that measures the overall performance of a binary classification model by plotting precision against recall at different threshold settings, providing a more accurate assessment of performance for imbalanced classes.
* Dataset used for customer-specific calculation: Shiraishi Y, Kataoka K, Chiba K, Okada A, Kogure Y, Tanaka H, Ogawa S, Miyano S. A comprehensive characterization of cis-acting splicing-associated variants in human cancer. Genome Res. 2018 Aug;28(8):1111-1125. doi: 10.1101/gr.231951.117. Epub 2018 Jul 16. PMID: 30012835; PMCID: PMC6071634.
* Baseline implementation: Predicting Splicing from Primary Sequence with Deep Learning. Jaganathan, Kishore et al. Cell, Volume 176, Issue 3, 535 - 548.e24

01

Optimized Setup

02

Customization

03

Assistants

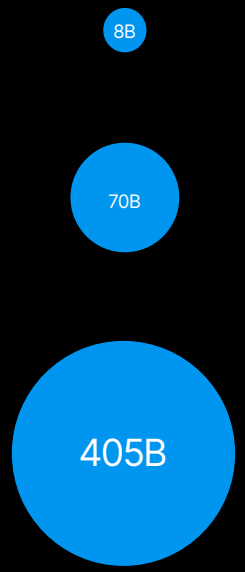
Build using natural language with Laila

Laila can form hypotheses, design experiments, and call tools to analyse results collaboratively with a human scientist


Demo screen

The Laila Series of AI Agents is built with Meta Llama 3.1

Model Sizes
in billions of parameters



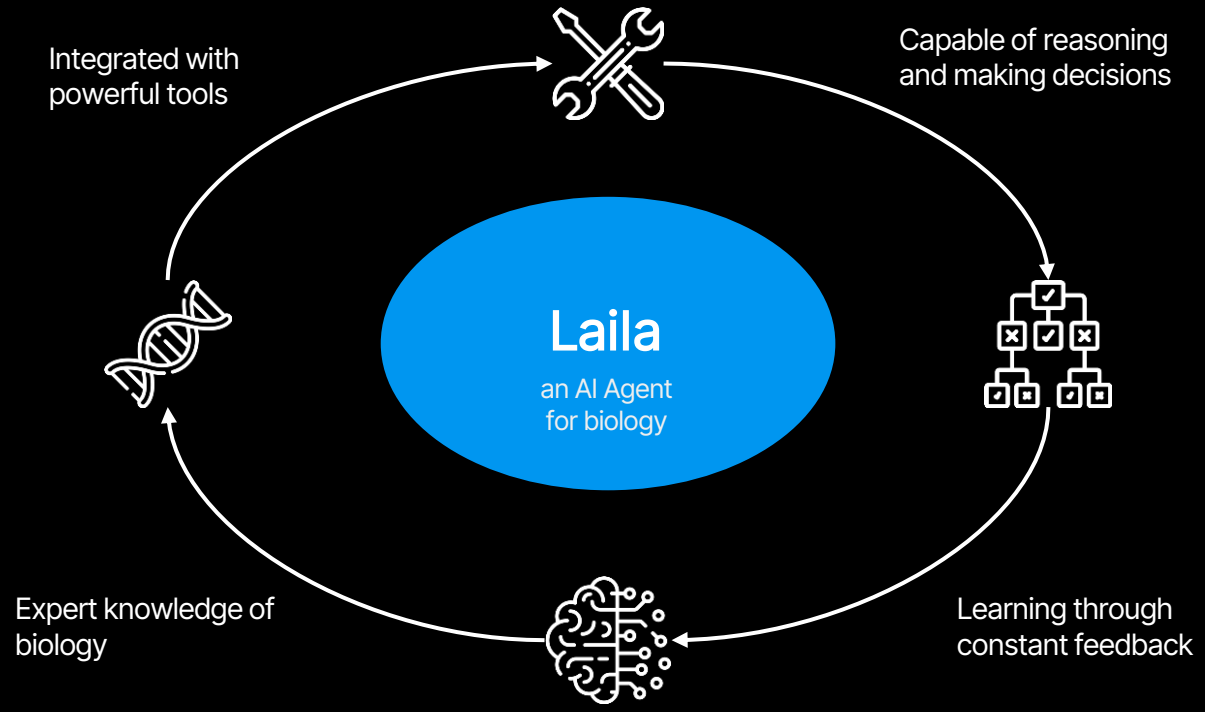
Model Versions
internally fine-tuned by InstaDeep

Llama-3.1-8B-Laila-fine-tuned

Llama-3.1-70B-Laila-fine-tuned

Llama-3.1-405B-Laila-fine-tuned

Laila is more than just a chatbot...



DeepChain

Features Models Try DeepChain Now

Accelerate your R&D Pipeline with Our Flagship AI Models

Industry-leading AI solutions for the life sciences

Get Started with DeepChain

Go to deepchain.bio to gain early access

Part II.

Deploying AI Across The Pipeline

Our Goal: Deploying AI end-to-end in our immunotherapy pipeline

AI-first Immunotherapy Platform

1. Immunohistochemistry → 2. DNA/RNA sequencing → 3. Proteomics → 4. Protein Design → 5. Lab Functional Validation

Histology

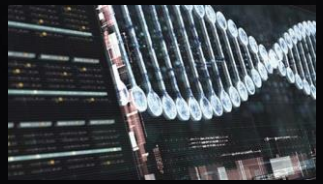
AI computer vision to improve speed and accuracy of tissue labeling

AI Vision

DNA

Sequence analysis and personalized genomic annotations

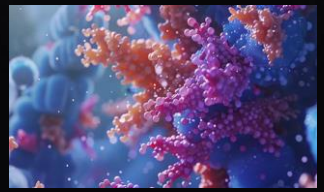
DNA LLMs



Proteomics

Leveraging AI for target discovery and analysis of the immunological landscape

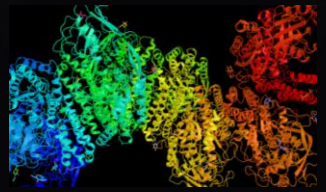
Protein LLMs



Protein Design

Developing assets for immunotherapy modalities (antibodies, cytokines, TCRs)

Protein LLMs



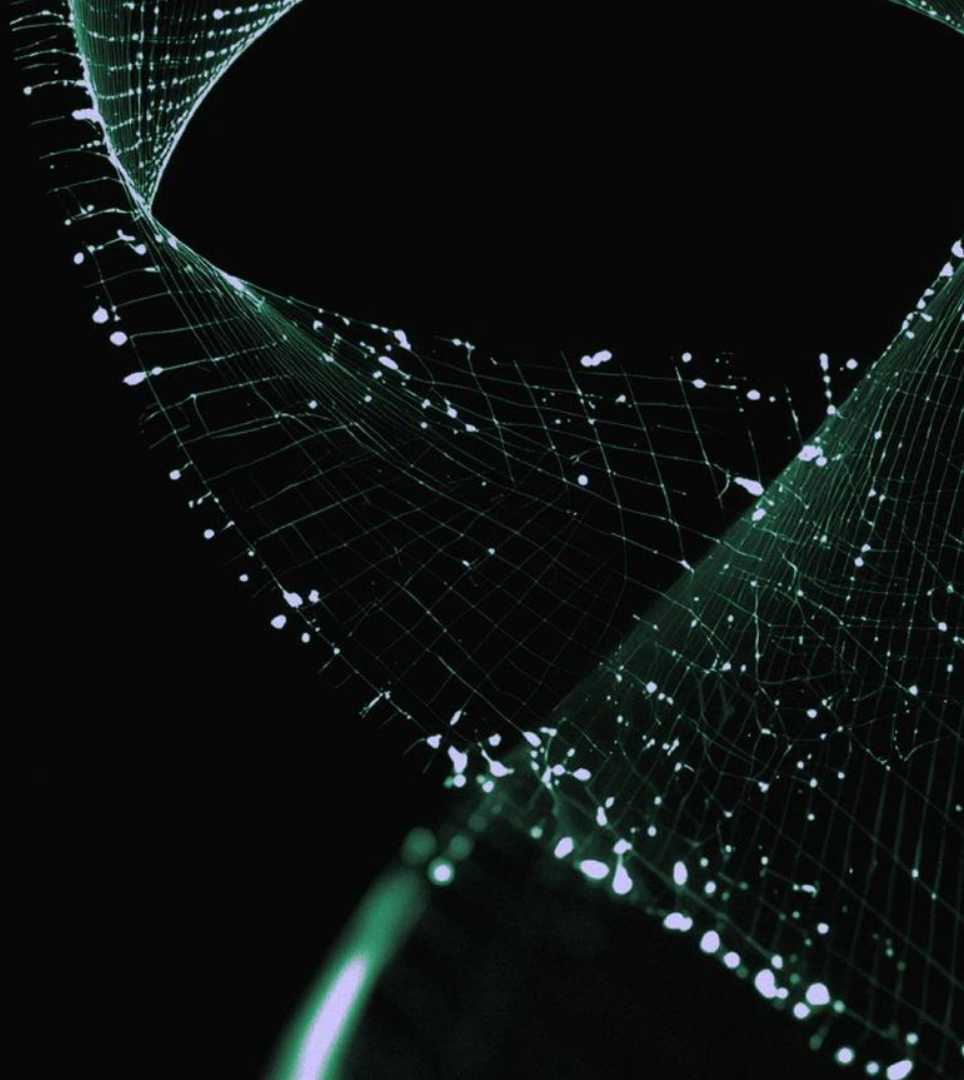
Lab

Instrument automation and quality control

AI Agent

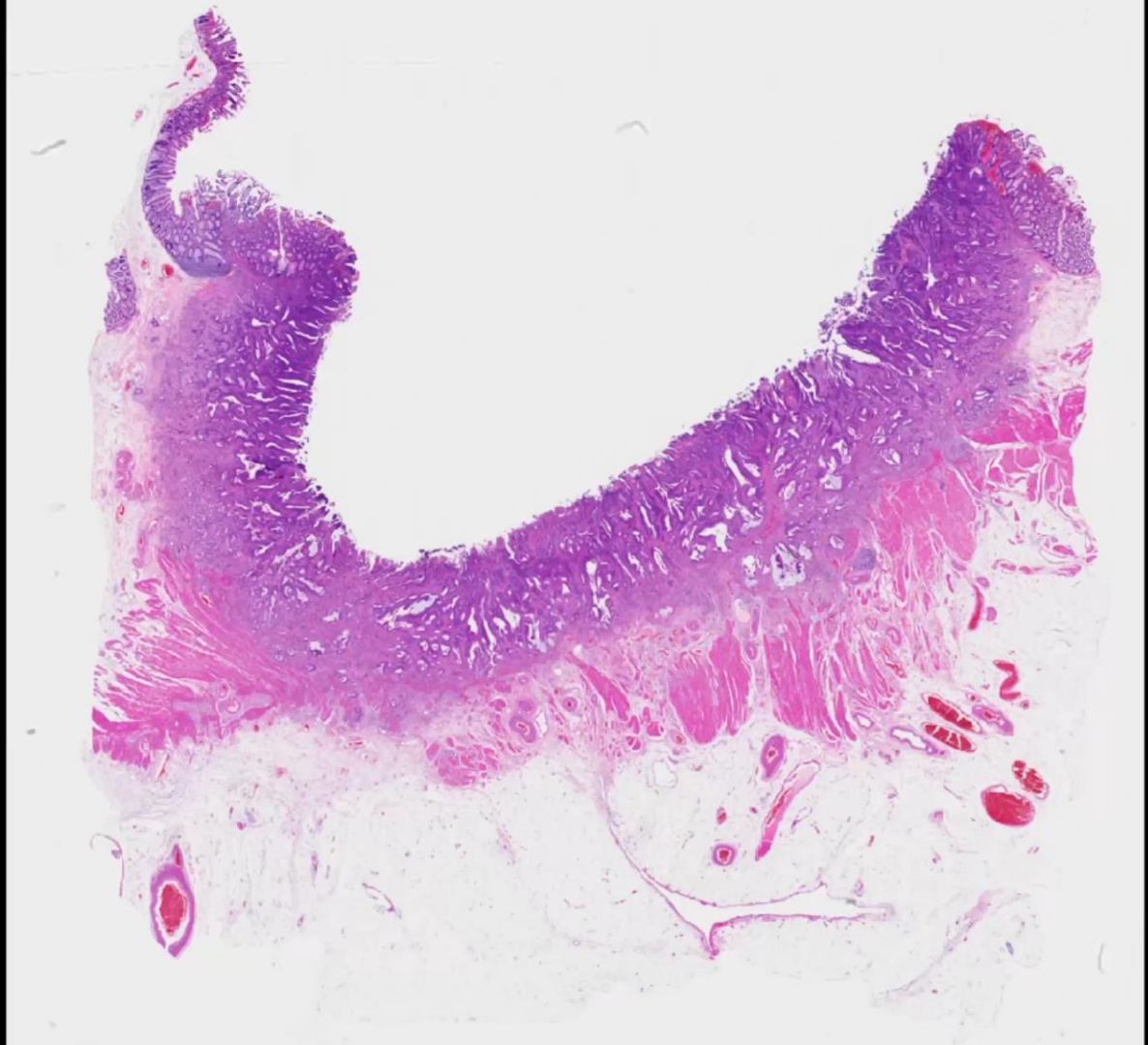
Step 1:

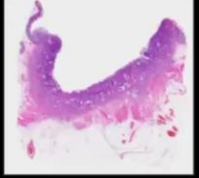
Histology



The Challenge

Pathologists face increasing workloads as demand grows for precise tumor and tissue analysis.





Source: Own Data

2 mm

16451.54, 6953.85 µm
157, 79, 178

Our Approach

Develop tools using state-of-the-art AI to enhance pathologists' workflows by producing faster and higher-quality annotations.

AI-Assisted Tissue Annotation Tool

Aiming to enhance Pathologists' Precision And Efficiency Through Human-AI Collaboration

5X Speed-Up

By increasing efficiency fivefold compared to manual annotation, our AI tool allows pathologists to complete annotations in a fraction of the time, optimizing resource utilization and accelerating research and development efforts.

Superior Annotation Quality

Enabling pathologists to refine annotations at different magnification levels in Whole Slide Images, resulting in higher-quality annotations.

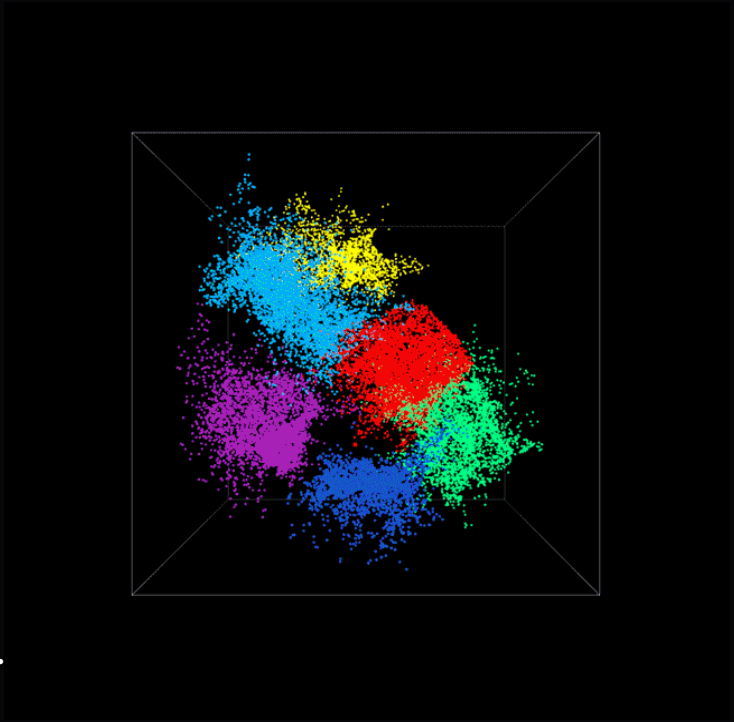
Whole Slide Image Segmentation Tool

From Classification To Segmentation

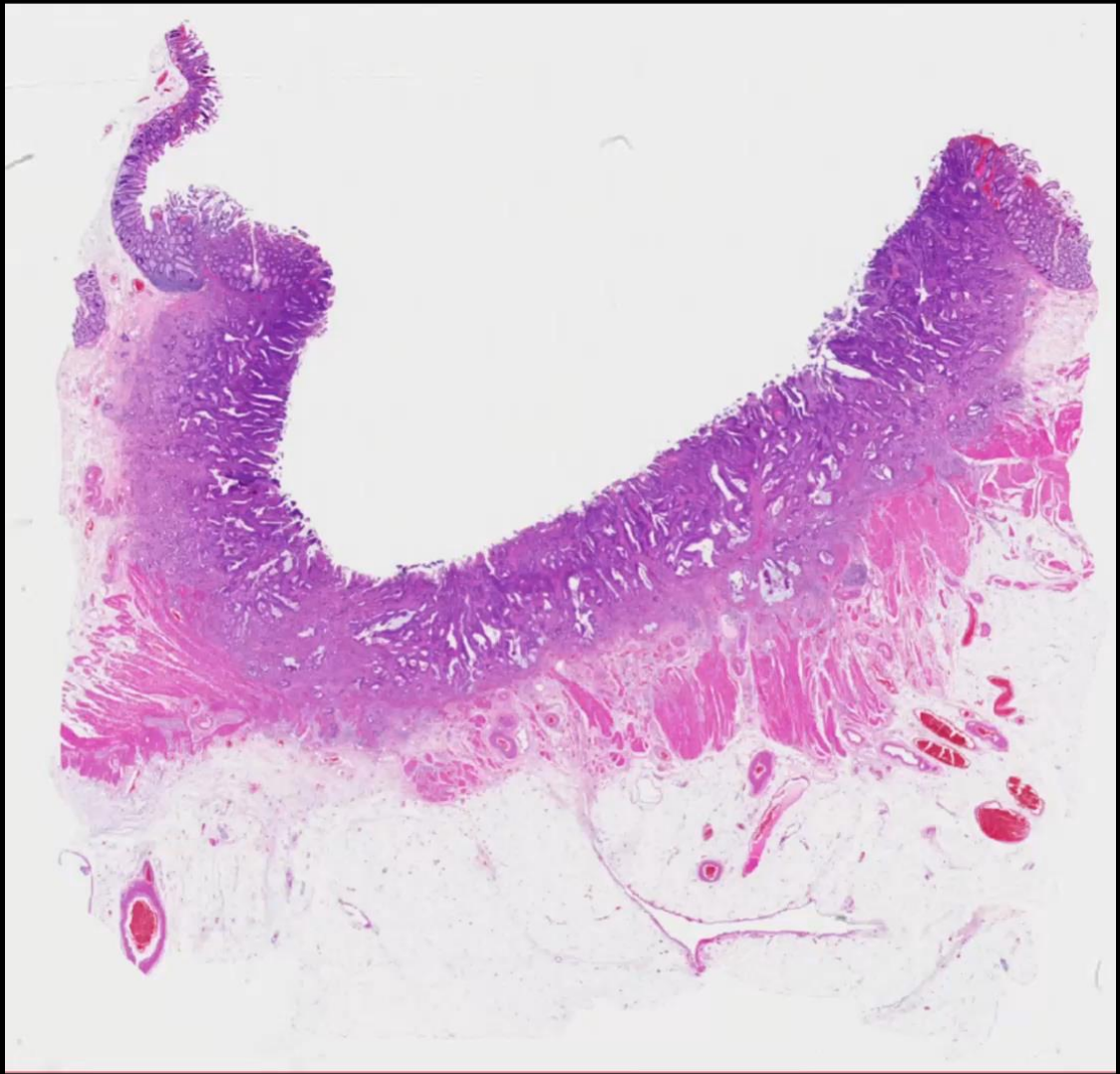
Use a state-of-the-art vision foundation model that we train specifically on pathology images.

Decompose the image into patches.

Transform the process from image segmentation to patch classification.



Source: Own Data



Source: Own Data

Scalable and Fast

By processing thousands of patches in parallel,
We deliver more than a 100 times speed-up compared to manual annotation.

Step 2:

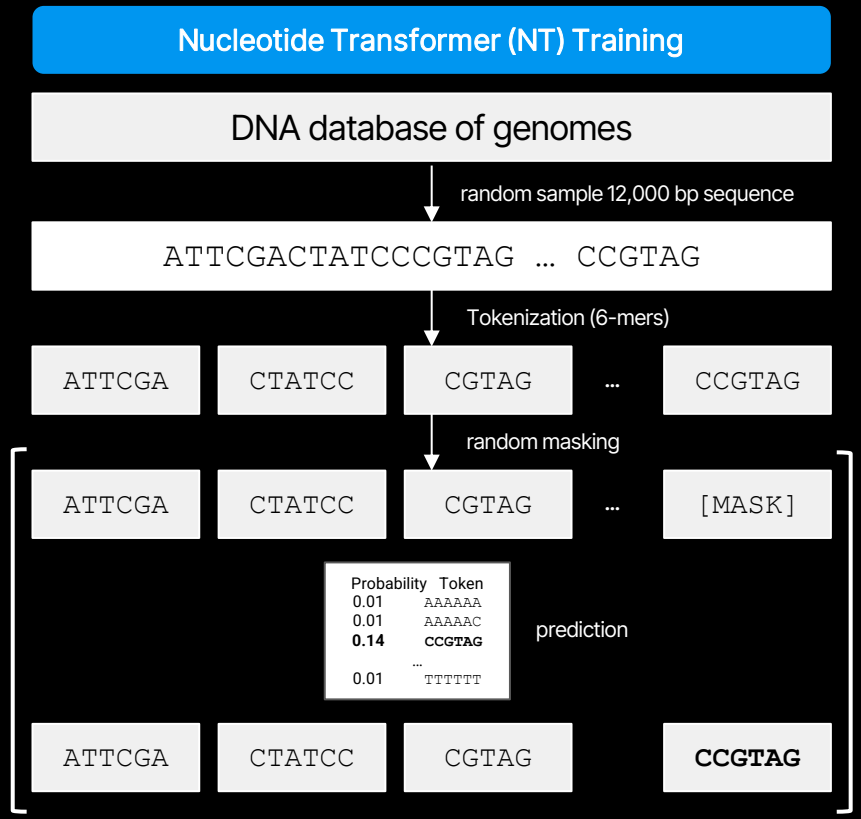
DNA Foundation Models at Nucleotide Resolution

Nucleotide Transformer: Self-Supervised Learning on Genomes

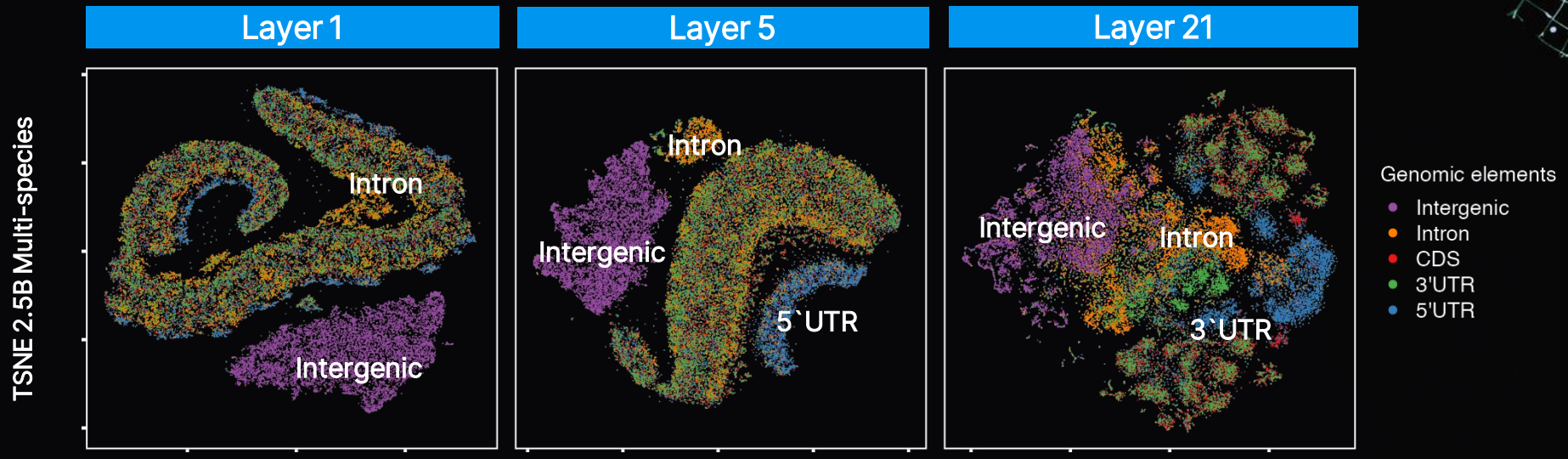
We believe **automated analysis and predictions from genome** sequences have the potential to **transform tomorrow's health care** and **agriculture.**

InstaDeep's Nucleotide Transformer Models

- *Architecture*: Masked Language Models (Bert-style training).
- *Datasets*: Trained on 5 datasets from different sizes with inter and intra-species variability from the whole tree of life.
- ***Nucleotide Transformers (NT)***
  - V1: 500M, 1B, 2.5B parameters (2022)
  - V2: 50M, 100M, 250M parameters (2023)
- ***Hardware***
  - Cambridge-1 Datacenter (collaboration with Nvidia)
  - TPUv4-1024 Pod (collaboration with Google Cloud)



NT Acquires Genomics Knowledge During Pre-Training



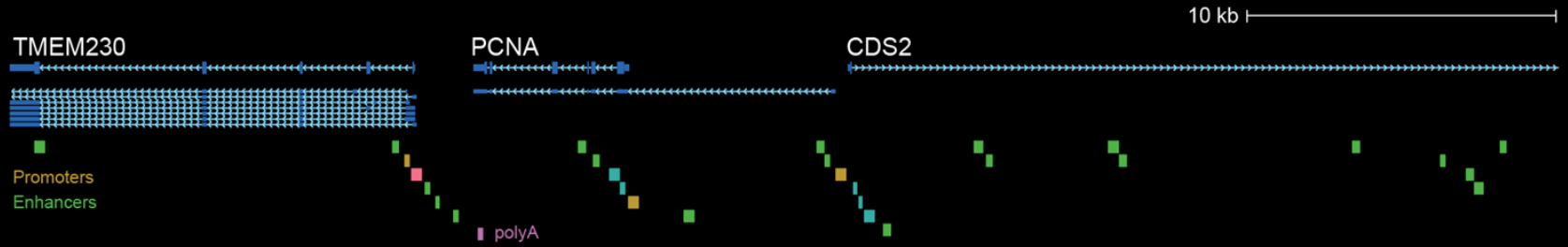
Even without supervision, information about **genomic sequence features is learned** in the "sequence representation"

***Source**: Dalla-Torre et al., Nat Methods* 2024 (in press)

SegmentNT: Inspiration from Computer Vision Segmentation Models

Computer Vision

Genomics



Source: https://techxplore.com/news/2020-05-deep-image-recognition-ability-self-driving.html

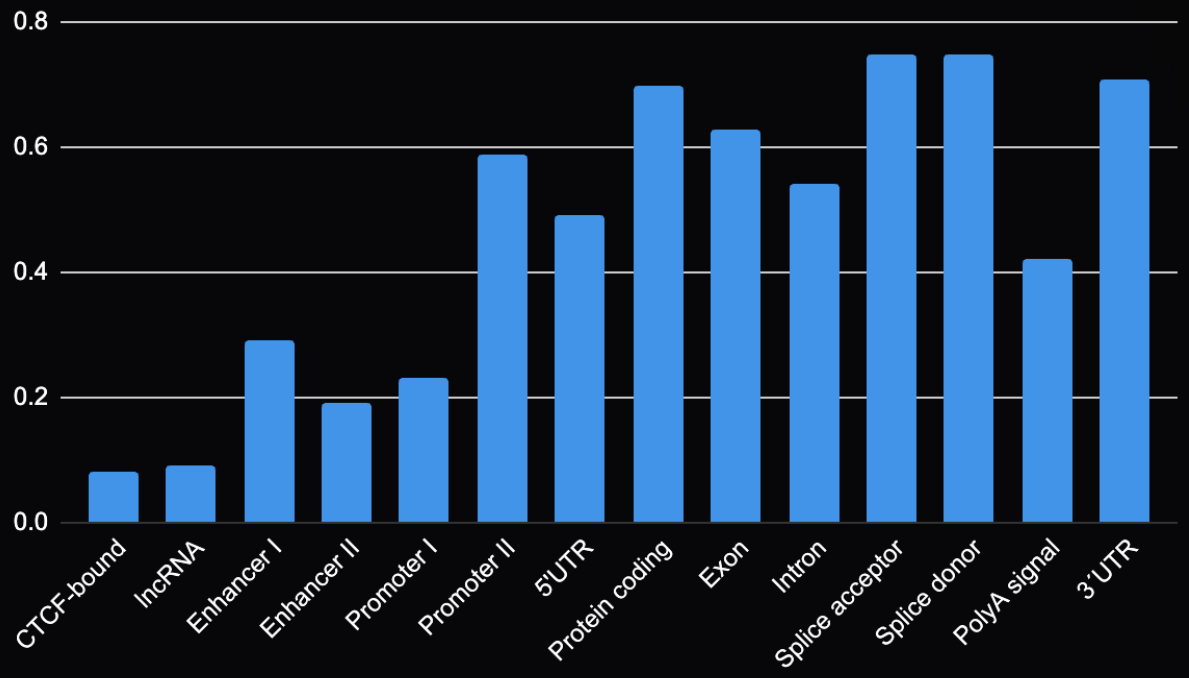
SegmentNT: Annotating the Genome at Nucleotide Resolution

We fine-tuned the Nucleotide Transformers on **2.5M** high-quality **gene and regulatory elements annotations**.

14 annotations per nucleotide (e.g. 700,000 predictions at 50kbp)

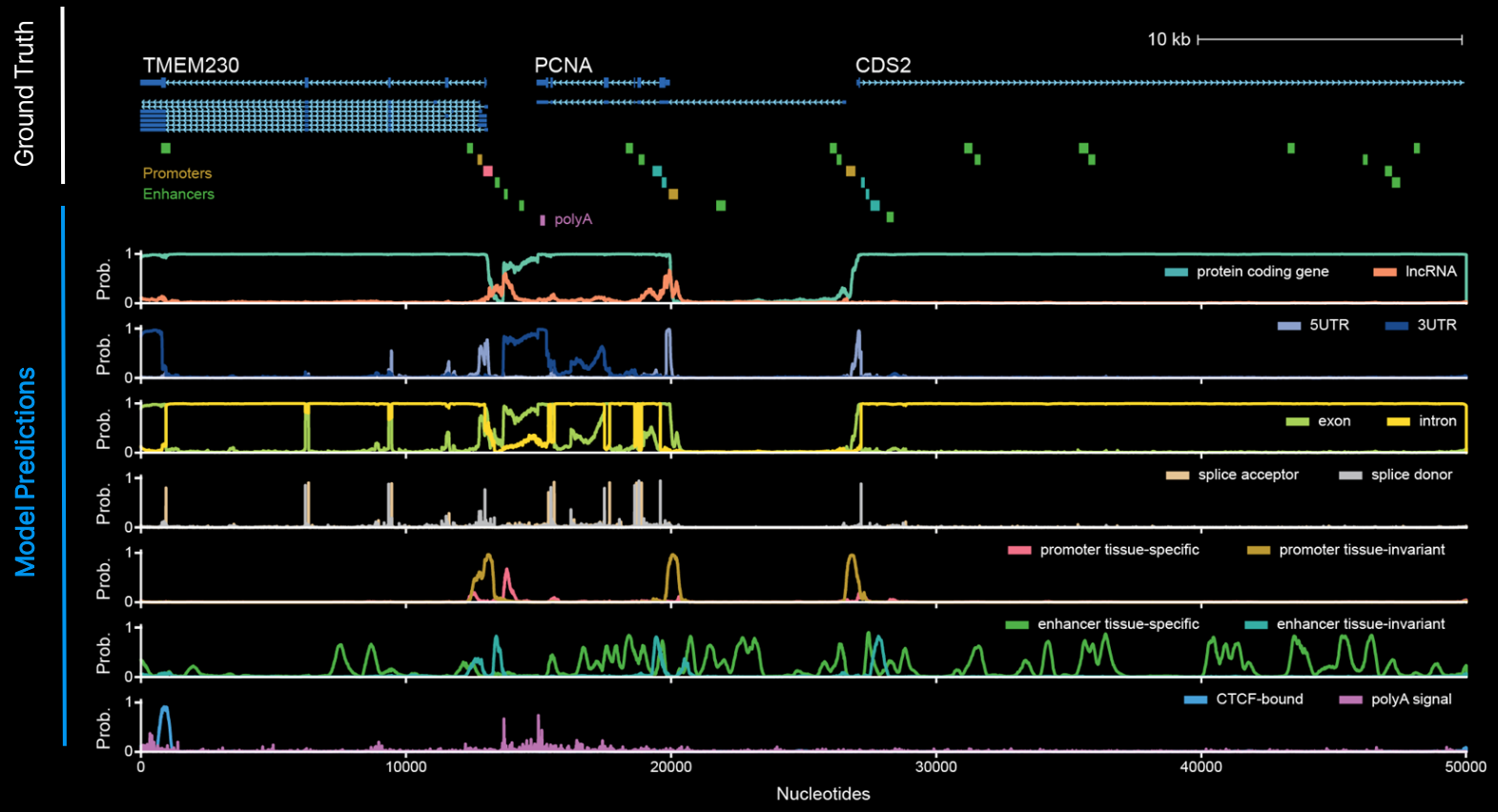
SegmentNT: Annotating the Genome at Nucleotide Resolution

The resulting SegmentNT model segments sequences up to **50kbp** with **state-of-the-art performance** for **splicing**, **gene finding** and **regulatory element detection.**



Source: adapted from de Almeida et al., 2024 (in revision)

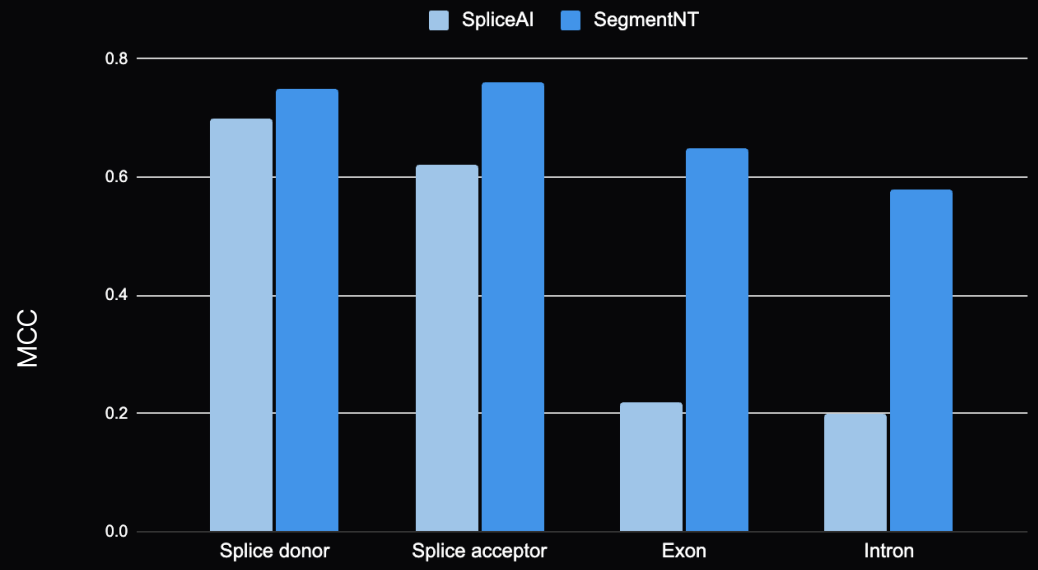
SegmentNT: 700,000 Accurate Predictions over 50kbp in less than a second



Source: de Almeida et al., 2024 (in revision)

SegmentNT is State-of-the-Art for Canonical Splicing Detection

Splicing is a biological process that **removes non-coding sequences** (introns) from a primary messenger RNA (mRNA) transcript and joins the coding sequences (exons) together to create a mature mRNA. **Dysregulated splicing** can be a **vulnerability in cancers**. SegmentNT **outperforms state-of-the-art SpliceAI** for splicing event detection.

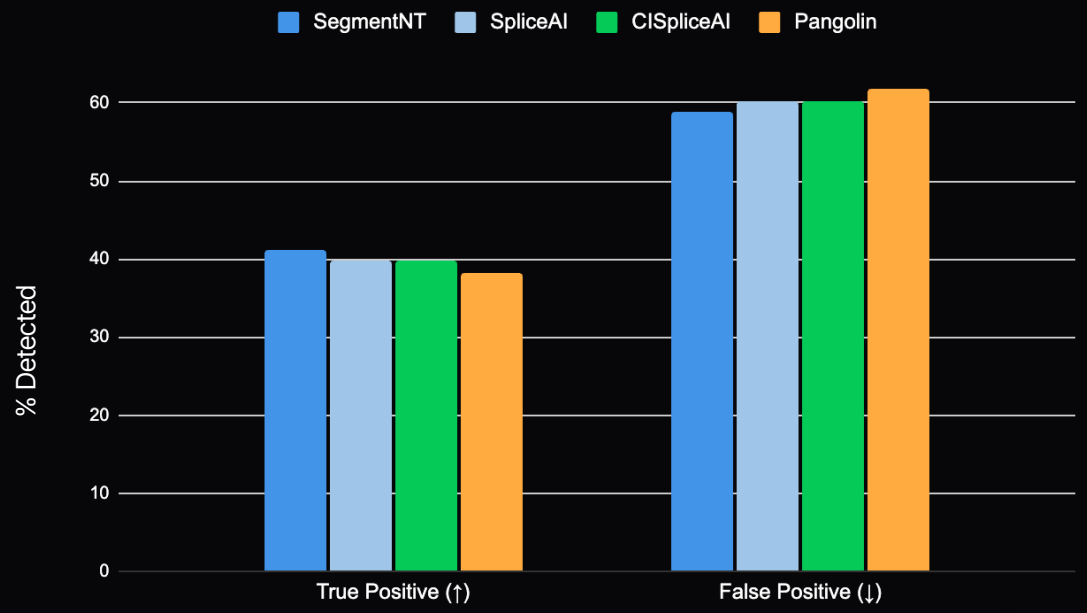


Test performance for splicing detection over full chromosomes on human reference genome

Source: de Almeida et al., 2024 (in revision)

Alternative Splicing Events Detection with SegmentNT

Alternative splicing events can disrupt protein production and cancer pathways and is associated with cancer development. We finetuned segmentNT to identify tumor antigen candidates from alternative splicing events, which represent potential targets for personalized cancer immunotherapies. After finetuning, SegmentNT can accurately predict alternative splicing events in cancer data.



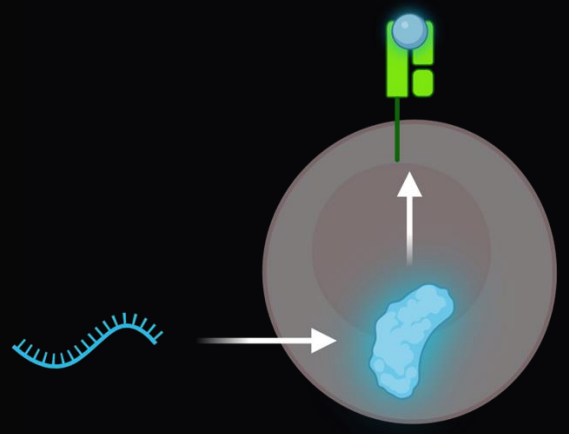
Test performance for 2,000 alternative splicing detection over cancer data (TCGA LUAD data)

Source: https://www.cancer.gov/tcga (data)

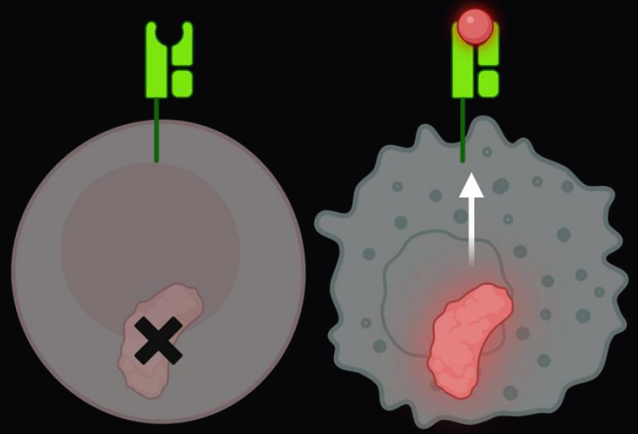
Step 3:

AI-Enhanced Proteomics for Target Discovery

Intracellular Proteins are Processed and Presented on MHC Complexes



T cell-targeting RNA vaccine

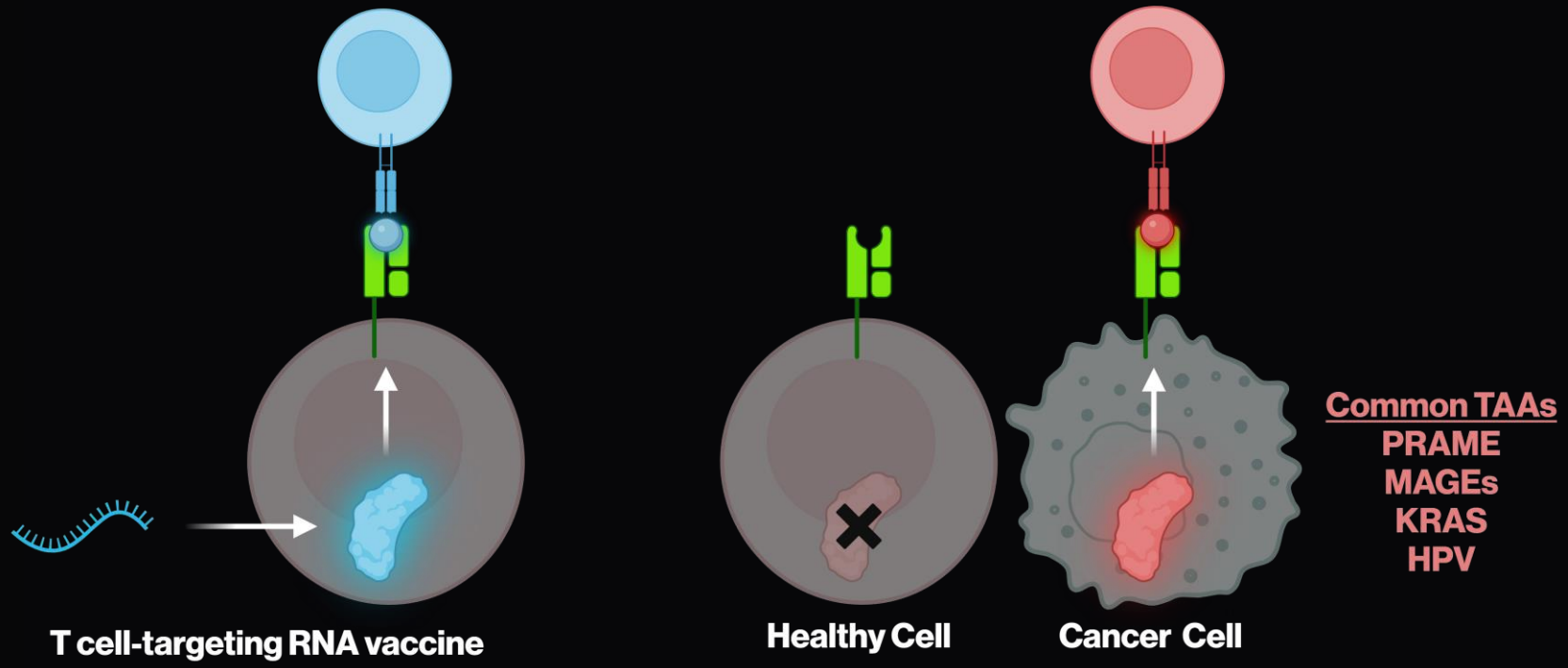


Healthy Cell

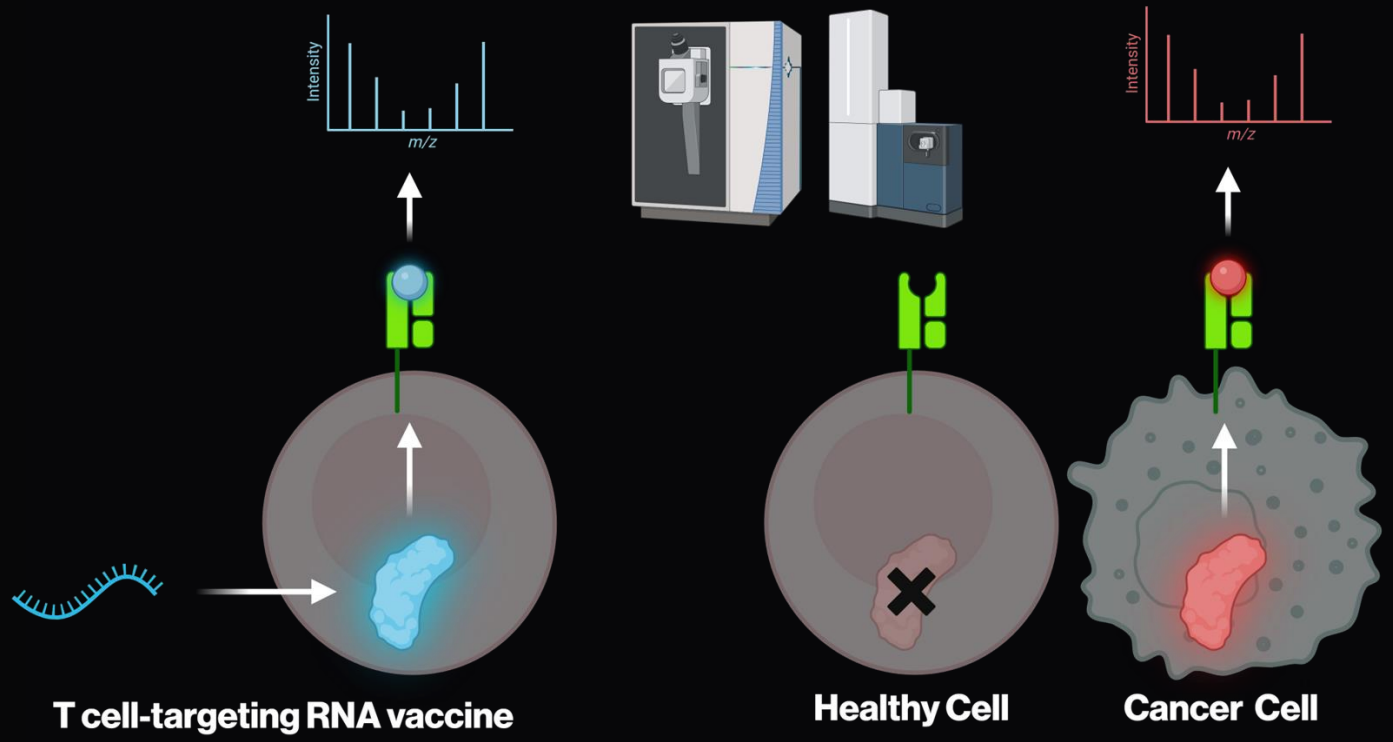
Cancer Cell

Common TAAs
PRAME
MAGEs
KRAS
HPV

MHC-presented Epitopes are Immune System's Window into the Intracellular Proteome

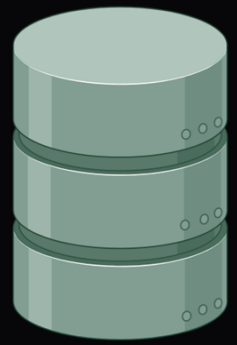


Mass Spectrometry is the Current State-of-the-art for Detecting, Identifying, and Quantifying MHC-presented Epitopes

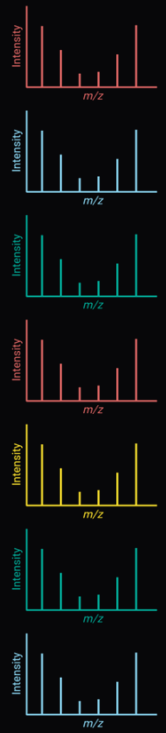


Common TAAs
PRAME
MAGEs
KRAS
HPV

BioNTech has a Massive Database of MS Validated MHC-bound Epitope Peptides from Studies Performed Internally and Externally



~200 million spectra
1.8 million peptides



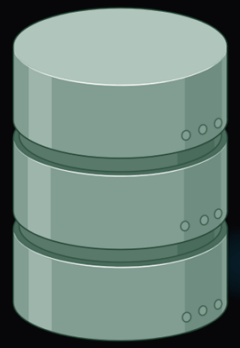
PEPTIDE → Not tumor specific

PEPTIDE → PRAME ✓

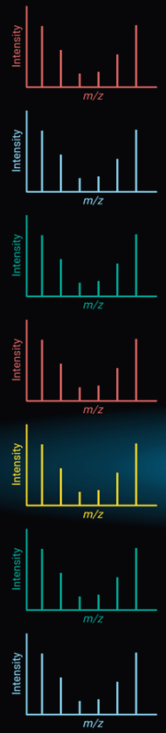
PEPTIDE → Not tumor specific

PEPTIDE → MAGE ✓

With the Power of AI, we can Dig Deeper into our Data to Identify Novel Therapeutic Targets



~200 million spectra
>>1.8 million peptides



PEPTIDE → Not tumor specific

PEPTIDE → PRAME

PEPTIDE → Not tumor specific

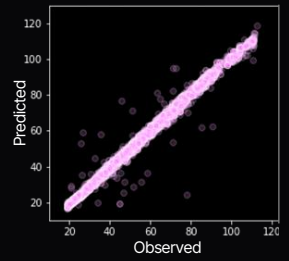
PEPTIDE → Novel Target

PEPTIDE → MAGE

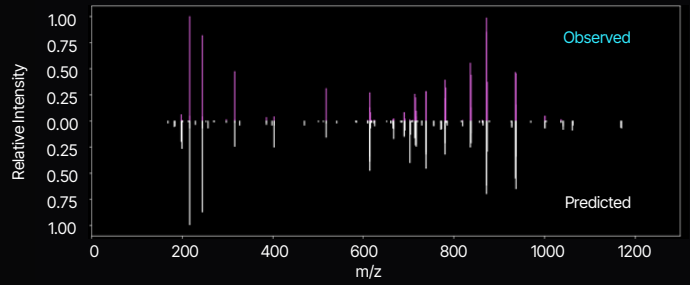
AI Maximizes our Ability to Discover Novel Cancer Targets

Up to 200% increase in recovered peptide IDs

Chromatographic Retention Time

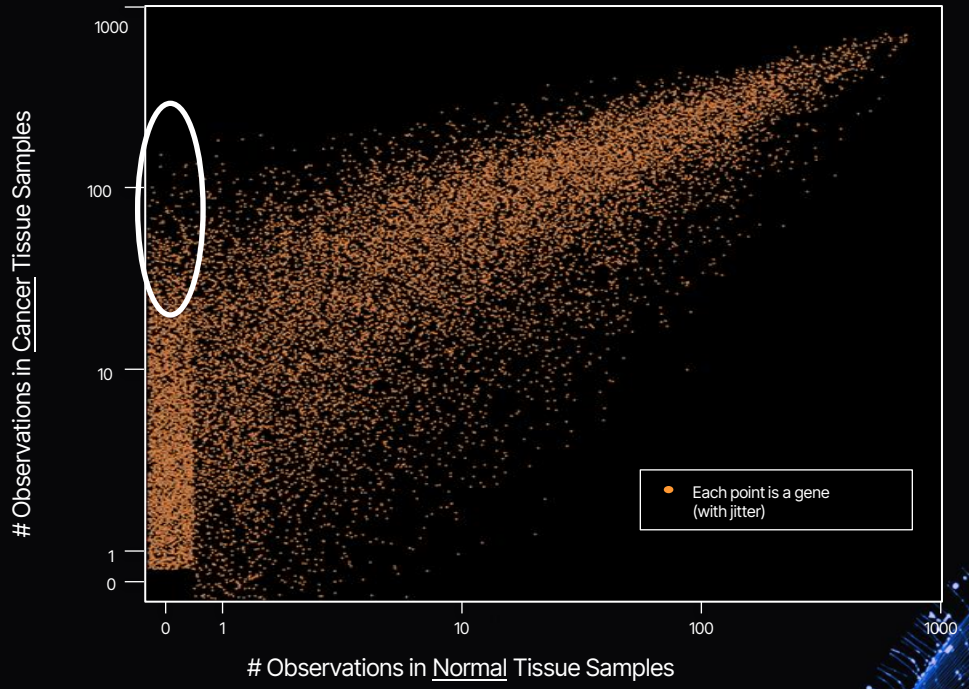


Signal intensities of peptide fragments



Source : Internal

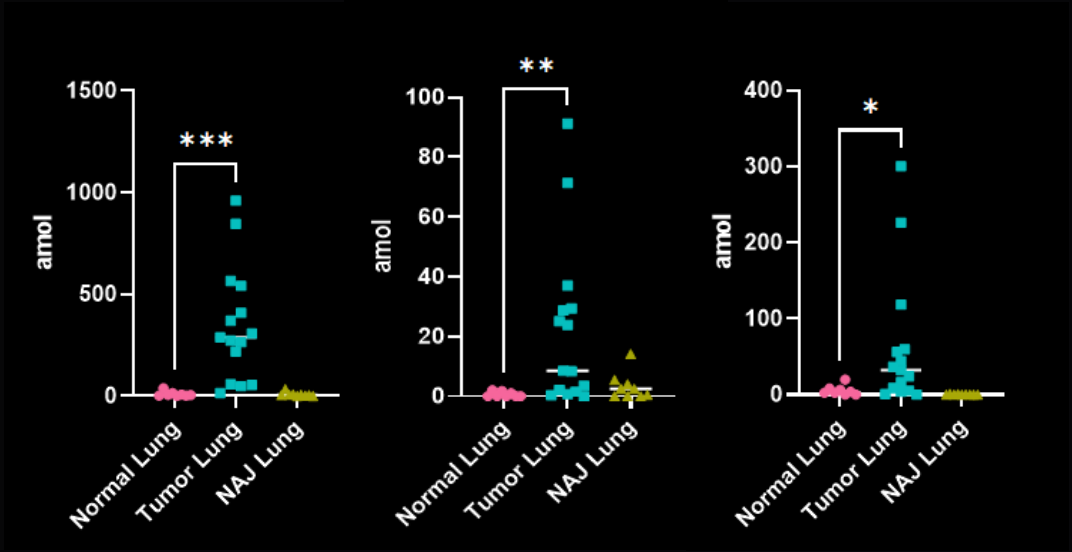
Identification of novel, tumor-specific peptides



Source : Internal

Targets are Validated with High-precision Mass Spectrometry

Lung Squamous Cell Carcinoma:
Example peptides validated using synthetic controls



Source : Internal

Validated targets are candidates for TCR-based therapies

Underway: Novel *in silico* approaches to discover and enhance TCRs

The Challenge of HLA Mass Spectrometry

55-75% of data cannot be mapped to a known human peptide

- LncRNAs
- Circular RNAs
- Non-canonical open reading frames
- Endogenous retroviruses
- Post-translational modifications
- ??

- Canonical human protein sequences

Traditional Mass Spectrometry Target Decoy Search

MS2 Spectrum

#1
#2
#3
#4
#5
#6
#7
#8
#9

Target Database
WQIPLCTVR
NRRRYTSSC
YVFGGLASA
FTASKTTW
...
ASLMPTYY

Decoy Database
RVTCLPIQW
CSSTYRRRN
ASALGGFVY
WTTKSATF
...
YYTPMLSA

MS2 Spectrum

#1
#2
#3
#4
#5
#6
#7
#8
#9

Peptide	Score
NRRRYTSSC	12.8
WQIPLCTVR	0.8
WTTKSATF	5.3
YVFGGLASA	19
ASLMPTYY	9.7
ASALGGFVY	2.1
RVTCLPIQW	11.6
YVFGGLASA	15.1
CSSTYRRRN	7.2

De Novo Peptide Sequencing

MS2 Spectrum

1.
2.
3.
4.
5.
6.
7.
8.
9.

Sequence to Sequence AI Model

Peptide

NRRRYTSSC

WQIPLCTVR

WTTKSATF

YVFGGLASA

ASLMPTYY

ASALGGFVY

RVTCLPIQW

YVFGGLASA

CSSTYRRRN

InstaNovo - *De Novo* Peptide Sequencing with Deep Learning

The approach

De novo peptide sequencing using deep learning. No database needed.

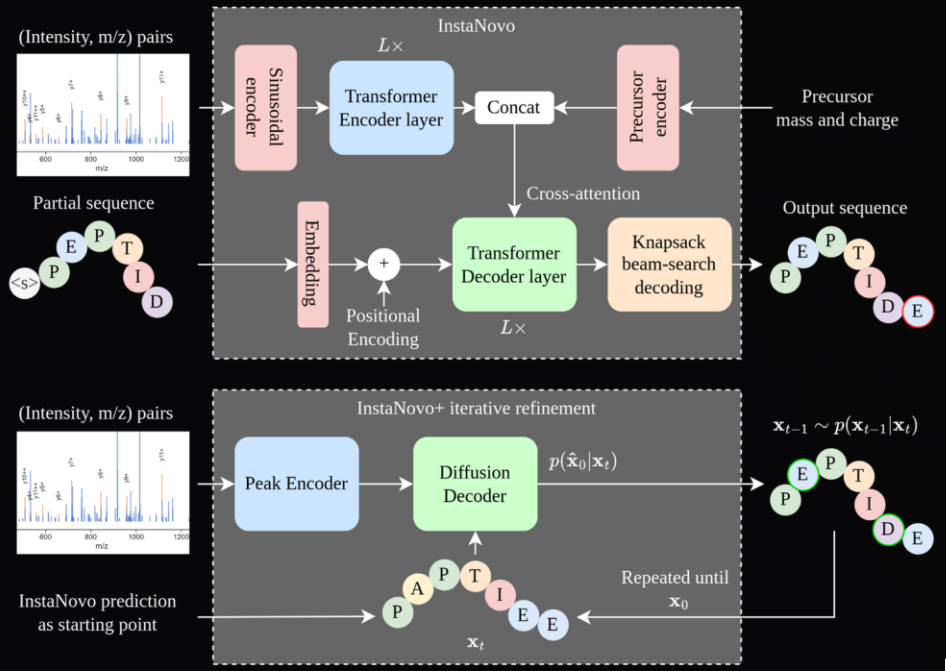
The dataset

Model trained on **28 million labeled spectra** matched to **742 thousand human peptides** from ProteomeTools project.

The models

InstaNovo
Autoregressive encoder-decoder transformer model with special MS2 spectrum encoder

InstaNovo+
Multinomial diffusion model to further improve performance using iterative refinement



Source: De novo peptide sequencing with InstaNovo: Accurate, database-free peptide identification for large scale proteomics experiments (https://www.biorxiv.org/content/10.1101/2023.08.30.555055v3)

InstaNovo - *De Novo* Peptide Sequencing with Deep Learning

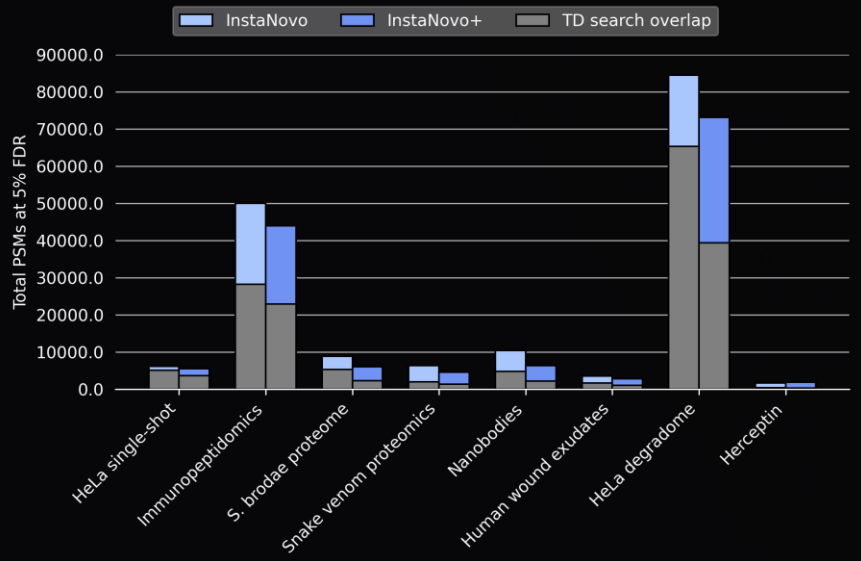
The results

- InstaNovo has performed well across most datasets
- Increases PSM rate in HeLa proteomes
- Expanded an immunopeptidomics dataset by 42%
- Found peptides from individual-specific mutations, splice variants, and post-translational modifications.
- Discovered new HLA peptides in immunopeptidome experiments

Preprint and code available

Preprint is available on **BioRxiv**
https://www.biorxiv.org/content/10.1101/2023.08.30.555055v3

Code is available on **GitHub**
https://github.com/instadeepai/instanovo



Source: De novo peptide sequencing with InstaNovo: Accurate, database-free peptide identification for large scale proteomics experiments (https://www.biorxiv.org/content/10.1101/2023.08.30.555055v3)

Step 4:

Protein Design: RiboMab™ Platform

Press Release

BioNTech and InstaDeep Announce Strategic Collaboration and Form AI Innovation Lab to Develop Novel Immunotherapies

25 November 2020

The strategic collaboration will focus on three core areas:

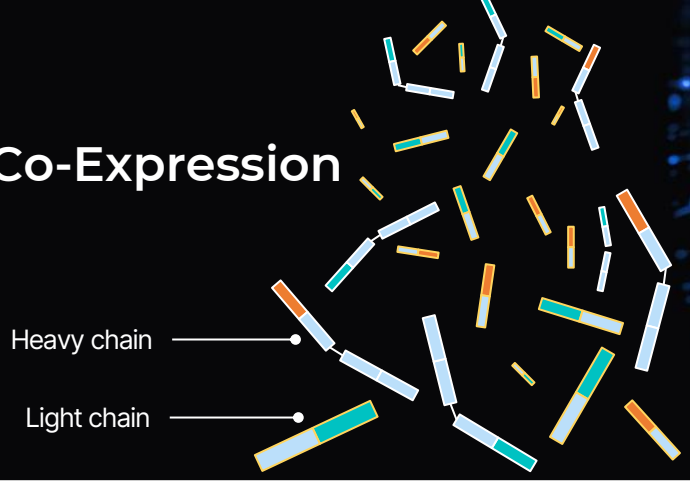
- **Novel Drug Design:** BioNTech is advancing a pipeline of novel mRNA-based vaccines and therapeutics and will apply InstaDeep's DeepChain™ protein design platform to engineer new mRNA sequences for protein targets, including for its RiboMab™ and RiboCytokine™ platforms, which use messenger RNA to encode antibodies and cytokines *in vivo*.

Source: https://investors.biontech.de/news-releases/news-release-details/biontech-and-instadeep-announce-strategic-collaboration-and-form/

Enabling Antibody Co-Formulation / Co-Expression

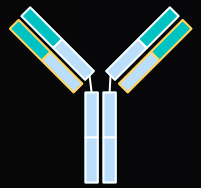
Co-expressed and bi-specific antibodies hold significant therapeutic interest.

However, these require precise pairing of heavy and light chains.

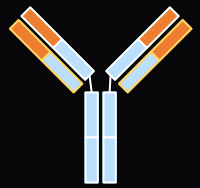


Correct Pairing

Antibody A
12.5%



Antibody B
12.5%



Functional form of co-expressed antibodies.

Mispairing: 75%

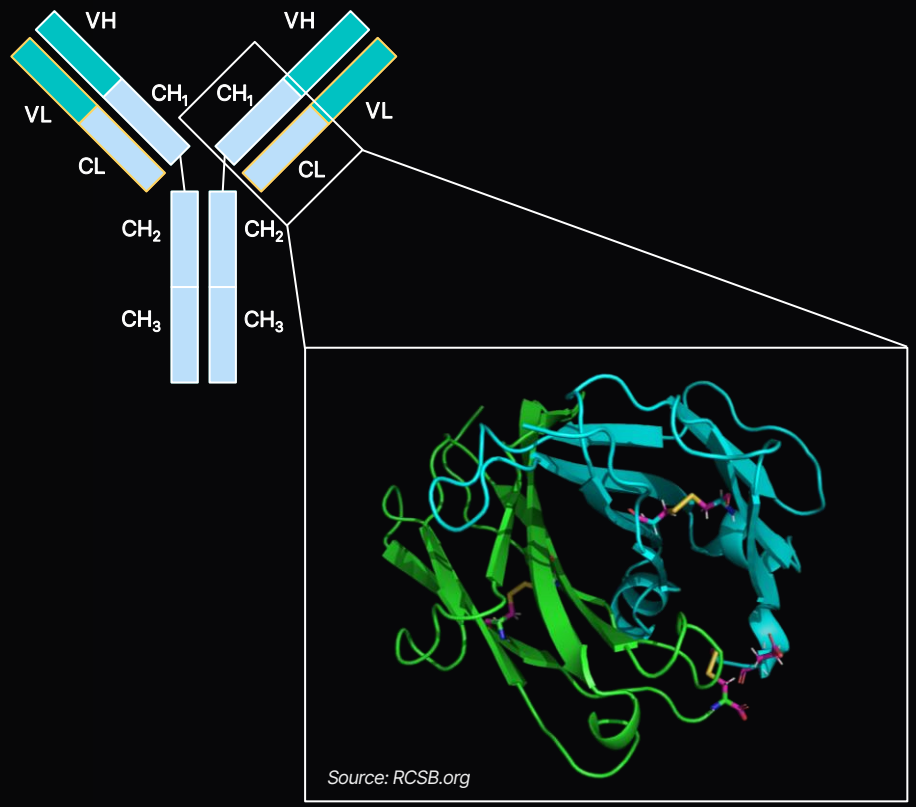
H-L Mispairing

Our goal: engineer the H-L interface to prevent mispairing.

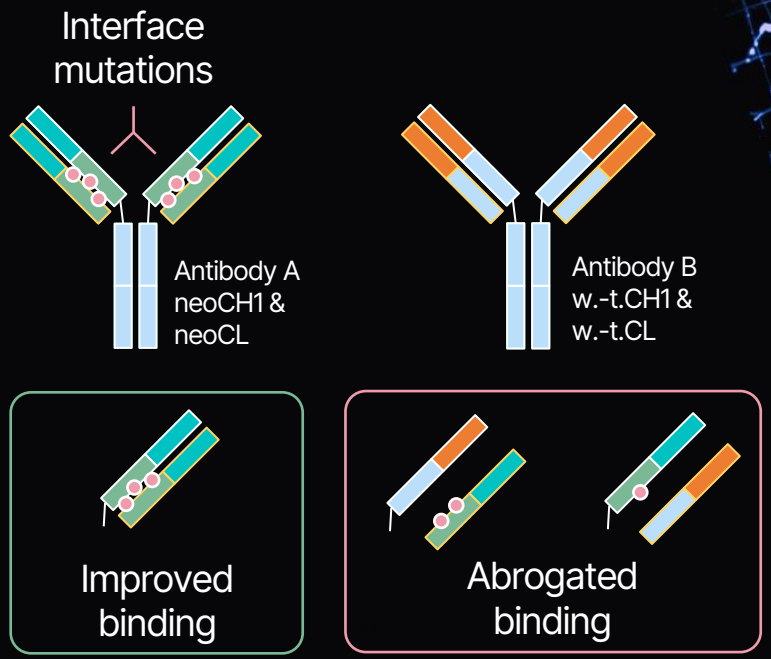
H-H Mispairing

H-H mispairing out of scope.

Our Protein Engineering Approach



We set out to introduce mutations to enforce orthogonality between neoCH1—neoCL v.s. wild-typeCH1—wild-typeCL.



Finding Optimal Orthogonal Mutations

A combinatorial multi-objective optimisation problem we could solve thanks to our DeepChain™ platform and an efficient *in silico – in vitro* feedback loop.

Binding energy estimations

For all correctly paired and mispaired complexes.

Mitigation of thermostability changes

For all both heavy and light chains.

Structural modelling

Of each interface mutation.

Key interaction understanding

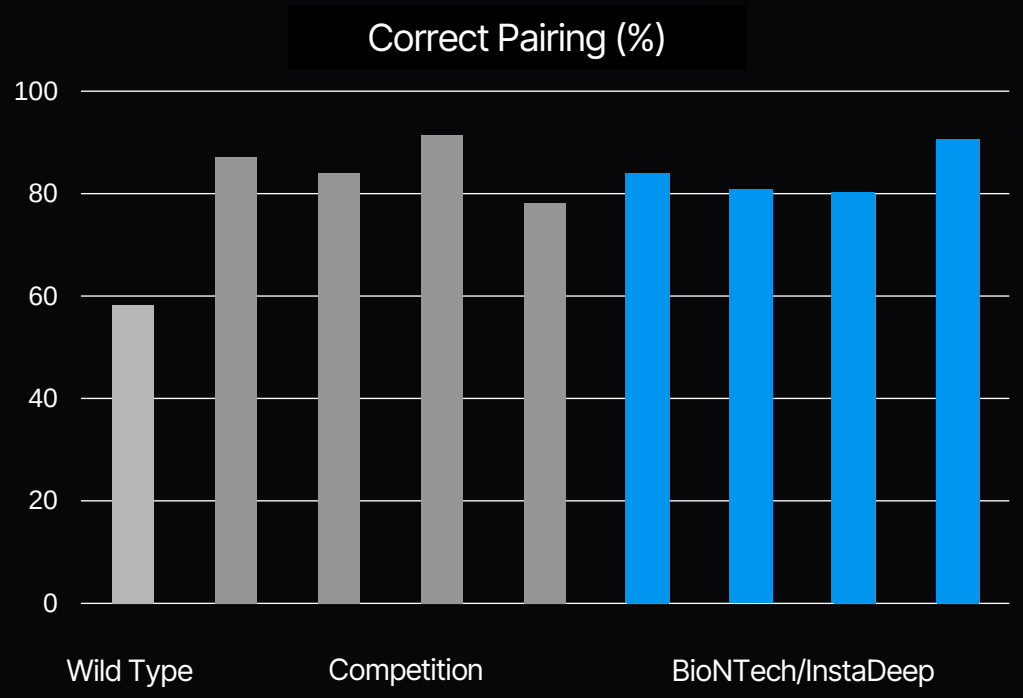
In depth knowledge of the physics of the interface.

RiboMab™ Results obtained with DeepChain™

>90% correct pairing

Matching the best patented designs on the market.

Functional activity of antibodies confirmed.

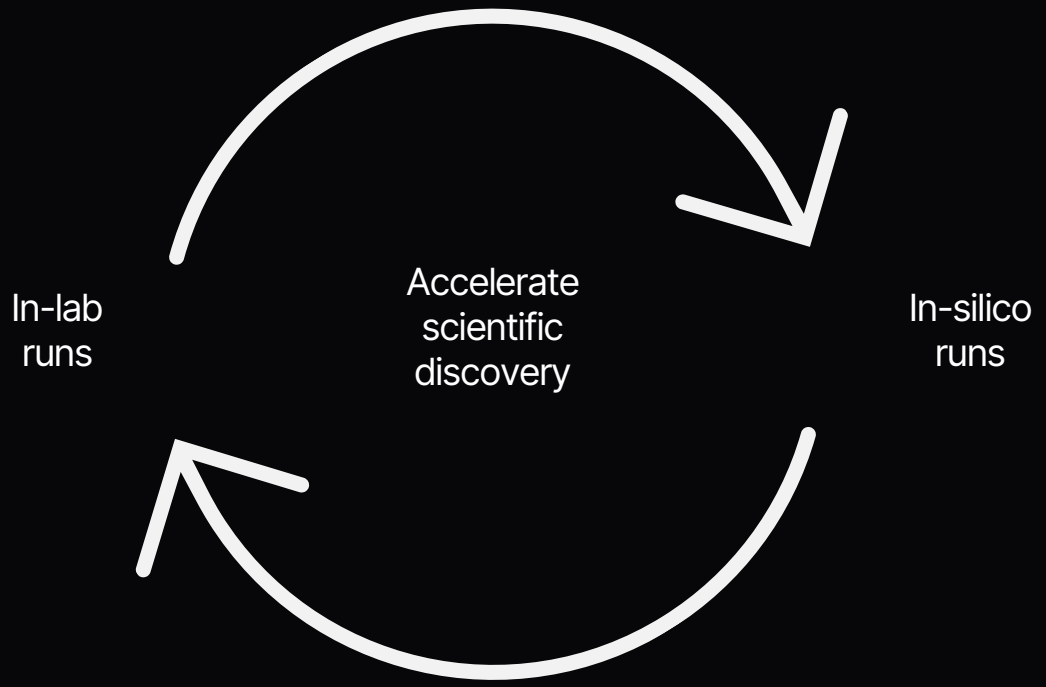


Source: Internal Data.

Step 5:

Lab Automation

Lab Automation Could Transform Research & Development



Challenges

Change

R&D is changing constantly

Complexity

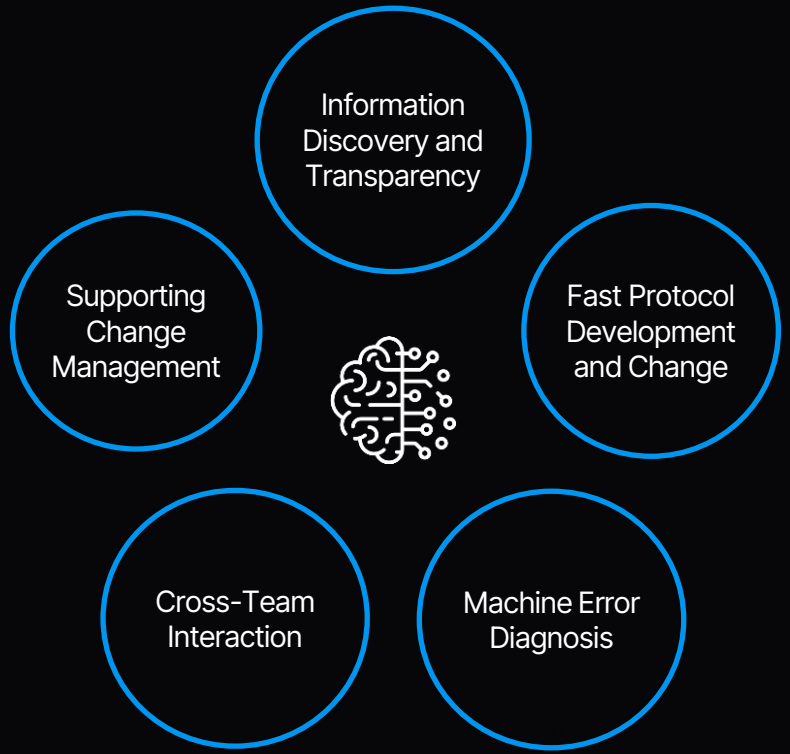
High complexity of science and automation

Transparency

Scientists need transparency and trust

Opportunities to Unlock Full Lab Automation with AI

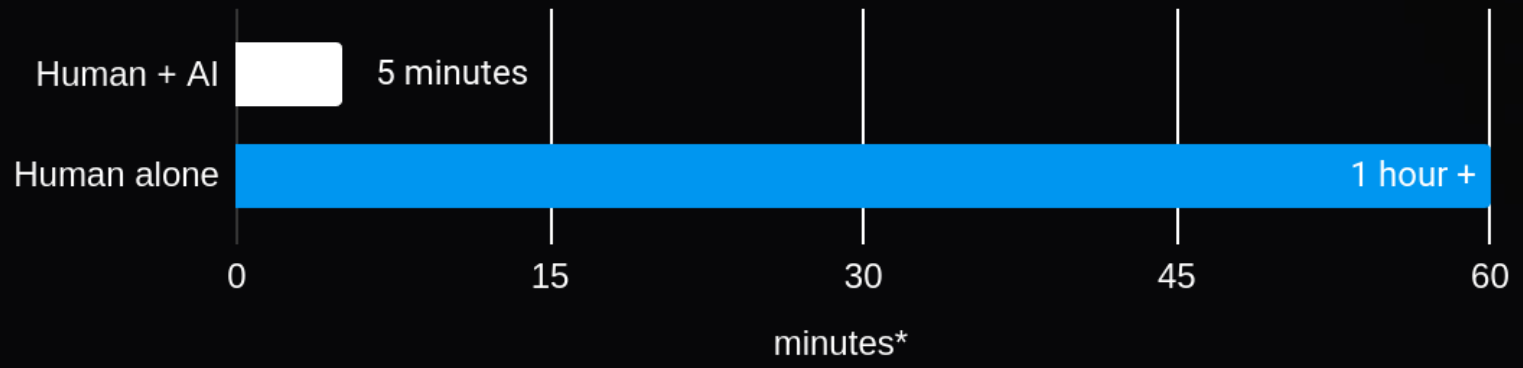
With the assistance of Artificial Intelligence, we see opportunities to overcome these challenges and unlock the full potential of laboratory automation



Demo

Increased Efficiency Across Laboratory Research Activities

Case Study: liquid handler error diagnosis



*Stated times are for an unexpected error

Lab Automation Demo – Future Outlook

Technology capability established

- AI-led Assay Information
- Vendor Agnostic Solution
- AI based Assay optimization
- DNA/ RNA Template optimization
- Interactive and natural language based
- Hiding Complexity of devices

Next Steps

- **Carve out different group requirements**
- **Connect to BioNTech's Digital R&D Backbone**
- **Scale up to other devices**

One more thing...

BIONTECH | InstaDeep™

AI Day Executive Summary

Ugur Sahin
Founder & CEO
BioNTech

Ryan Richardson
Chief Strategy Officer
BioNTech

Karim Beguir
CEO
InstaDeep

BIONTECH | InstaDeep™

Thank You!
THE END