Current application of

# Artificial Intelligence

## Tools and Resources in Biomedical Research

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# Why AI? Why now?

Current biomedical research is a **petabyte factory**

| | | | |
|---|---|---|---|
| **30M+**<br>**PubMed articles**<br>**~4.000 new/day** | **150 GB**<br>**per WGS genome**<br>**raw sequencing** | **10 yrs**<br>**$2.6B**<br>**drug development** | **x100**<br>**Data growth in omics over the last decade** |

Biomedical research generates more data than human can process

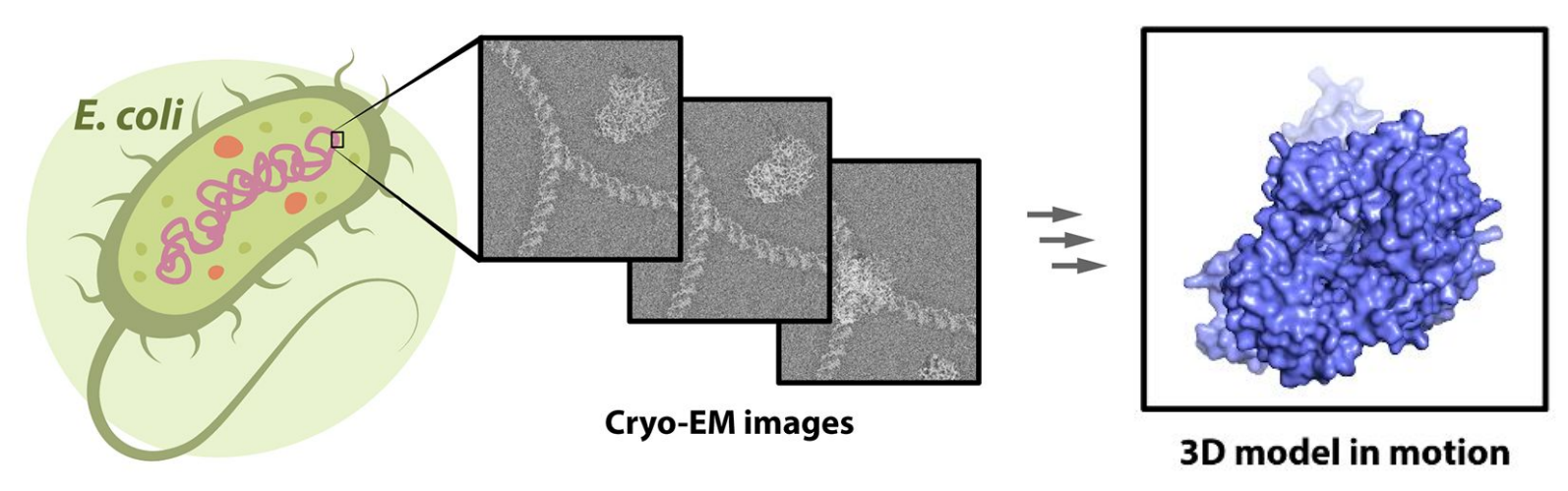
**HPC + AI bridges the gap between data and scientific insight**

# Why AI? Why now?

## Ex. Cryo-electron microscopy (cryo-EM)

**Nobel Prize 2017**

A single data acquisition session using a high-end microscope can generate **several terabytes** of raw data in a **single day**






Baldwin PR *et al*. Big data in cryoEM: automated collection, processing and accessibility of EM data (2018) doi: 10.1016/j.mib.2017.10.005.
https://morgridge.org/feature/cryo-em-primer/

# Paradigm change

## Shifting from Deterministic Analysis to AI-Driven Insights

**Classical bioinformatics**

- **Deterministic** pipelines
- **Structured** data
- **CPU-**intensive

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**AI + Bioinformatics**

- **Stochastic** pipelines
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**Adapt** & **Re-think** our **tools**

# The AI Toolkit

## A methodology-first view of current algorithmic families

CPU CLUSTER

### Classical ML

RF, SVM, XGBoost

Biomarker discovery, clinical risk scores and feature selection

GPU

### Deep Learning

CNN, RNN, Transformers

Medical imaging analysis, basic sequence modeling and EHR structured data

GPU + Large RAM

### Graph Neural Nets

GNNs, DeepGraph

Drug-target interaction, knowledge graphs and protein-protein networks

High VRAM

### Generative AI

GAN, VAE, Diffusion

Drug molecule design, protein engineering and synthetic data generation

Multi-GPU

### Large Language Models

Bio-LLMs, scGPT, Geneformer

Literature mining, clinical NLP and foundational models

HYBRID CPU + GPU

### Reinforcement Learning

DQN, PPO, AlphaZero

Experimental design automation, adaptive clinical trials and robotics

# Workload archetypes

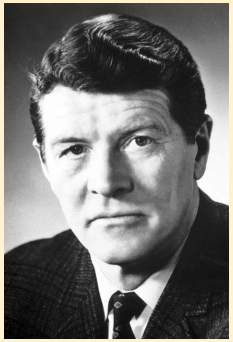
**Hardware-centric classification for high-performance biomedical workloads**

| | Type | Example Models | Critical Hardware | Execution pattern |
|---|---|---|---|---|
|  | **Bio sequences** | **AlphaFold / DNABERT**<br>Proteins & Genomics | GPU<br>RAM<br>Flash Storage | CPU heavy prep +<br>GPU modeling |
|  | **Computer vision** | **MONAI**<br>Tumor Segmentation | GPU<br>High Speed NVME | Cold training /<br>Massive inference |
|  | **NLP (Bio-LLMs)** | **scGPT / PubMedBERT**<br>EHRs & Literature | GPU<br>Text I/O | Frequent, dynamic<br>fine-tuning |
|  | **Digital Chemistry** | **GNNs / DiffDock**<br>Drug discovery | GPU<br>RDMA networking | Parallel screening /<br>Job arrays |

# AlphaFold

Bio sequences

## Solving the 50-year Protein Folding Challenge using AI



**Chemistry Nobel Prize**

**1972**

**Christian Anfinsen**

The **sequence** of amino acids, in **itself**, **determines** the way **the chain folds** itself and that **no additional** genetic **information** is **required** in this process.

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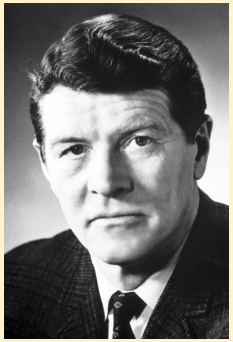

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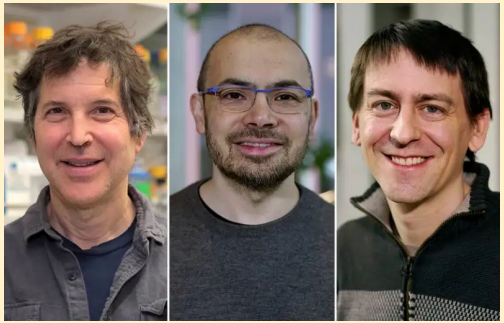

**Chemistry Nobel Prize**

**2024**

**Baker, Hassabis, Jumper**

AlphaFold2 **predicted** the 3D structure of **+200 million proteins** —virtually all known to science— **achieving in years** what would have taken **centuries of** manual lab **work**.

# AlphaFold: how does it work?

Bio sequences

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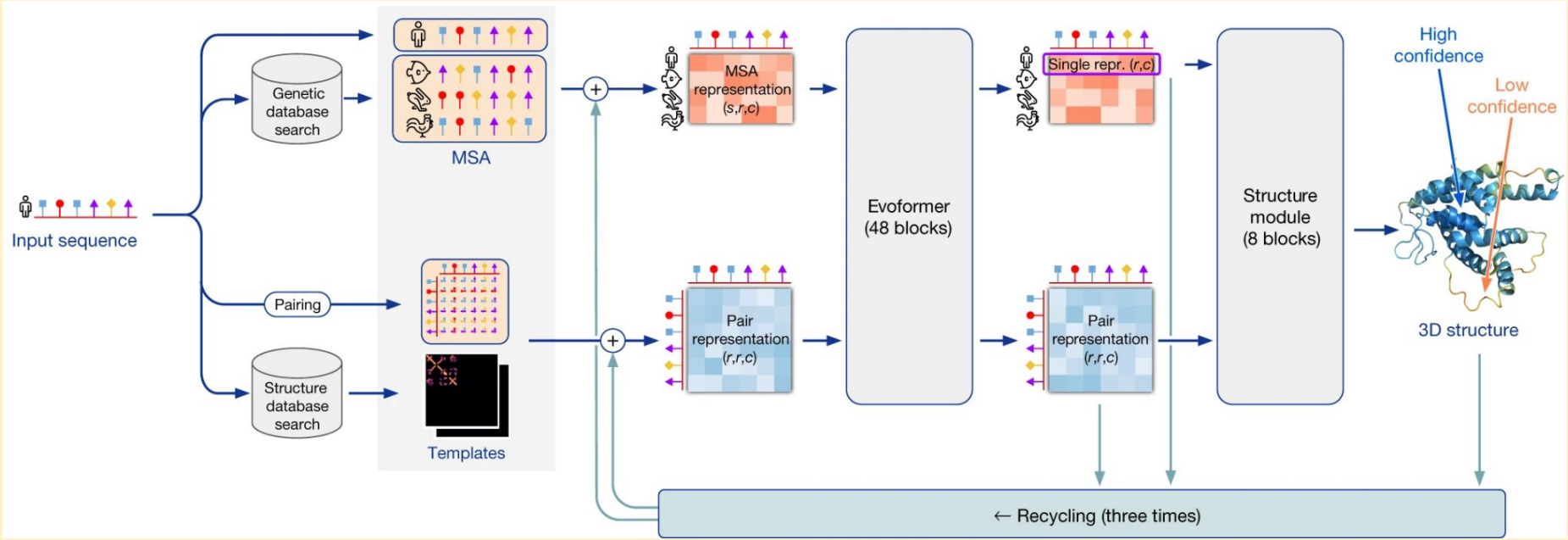




Jumper, J., Evans, R., Pritzel, A. et al. Highly accurate protein structure prediction with AlphaFold. Nature 596, 583–589 (2021). https://doi.org/10.1038/s41586-021-03819-2

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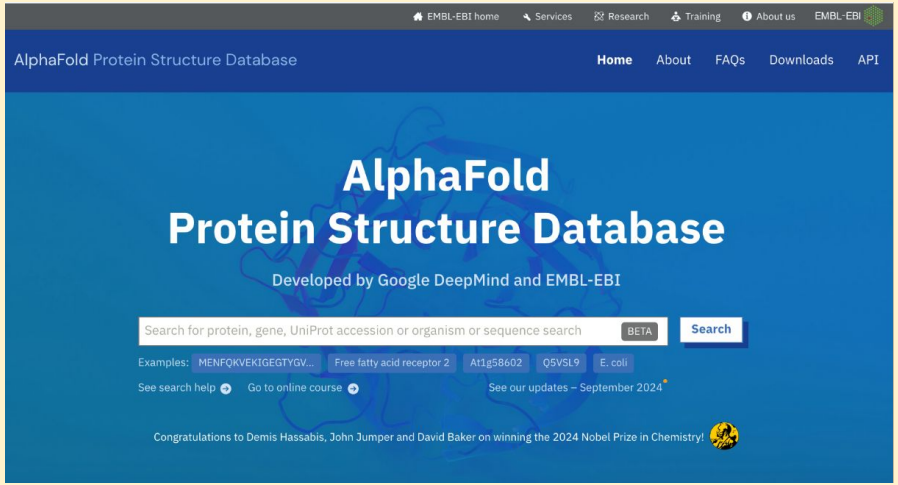
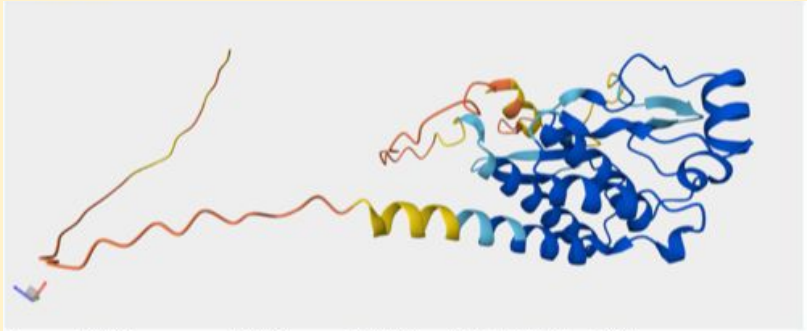


This work is a major step forward, but **it's not a solution**



Jumper, J., Evans, R., Pritzel, A. et al. Highly accurate protein structure prediction with AlphaFold. Nature 596, 583–589 (2021). https://doi.org/10.1038/s41586-021-03819-2

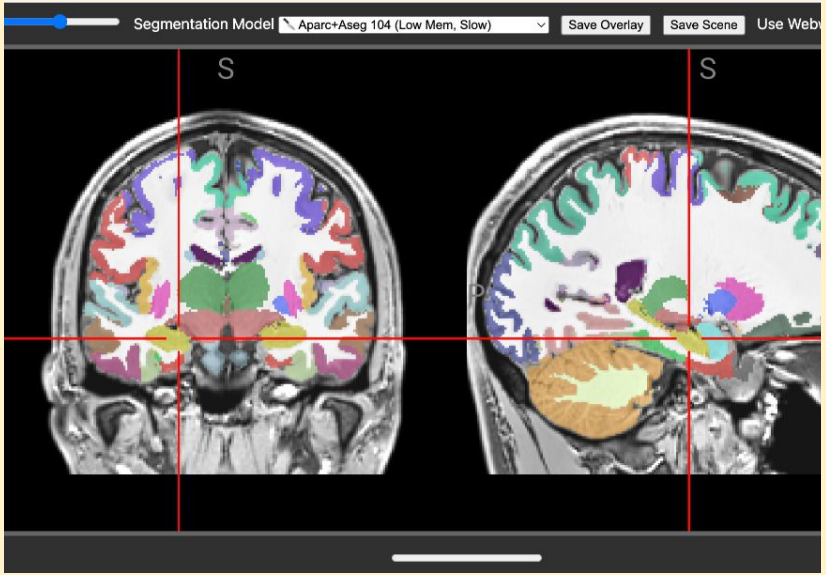
# Medical Open Network for AI

Computer vision

## MONAI: Bridging AI & Healthcare

**Based on PyTorch**

**Tools** & **libraries** for **developing**, **training** and **deploying** AI models in medical imaging applications (**segmentation**, **classification** & **registration**)






Plis, S. M., Masoud, M. et al. (2024). Brainchop: Providing an Edge Ecosystem for Deployment of Neuroimaging Artificial Intelligence Models. Aperture Neuro, 4, 2024. https://doi.org/10.52294/001C.123059

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Computer vision

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### MONAI Label

Create **training datasets** and build AI **annotation** models

### MONAI Core

Specialized infrastructure to **build** AI-driven medical imaging **pipelines**

### MONAI Deploy

**Simplify deployment** in existing medical infrastructure



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Preference for **turnkey** commercial **solutions** for faster deployment.



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Using **open source frameworks** to **prevent** "reinventing the wheel" with each imaging project



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# Foundational models and LLMs

NLP
(Bio-LLMs)

## Training a ‘Jack-of-all-trades’ model

**Before**

A **different dataset**
and a
**different model**
for each task

Greater **amount** of **data** required per task !!



Fei Guo *et al.*, Foundation models in bioinformatics, National Science Review, Volume 12, Issue 4, April 2025, nwaf028, https://doi.org/10.1093/nsr/nwaf028

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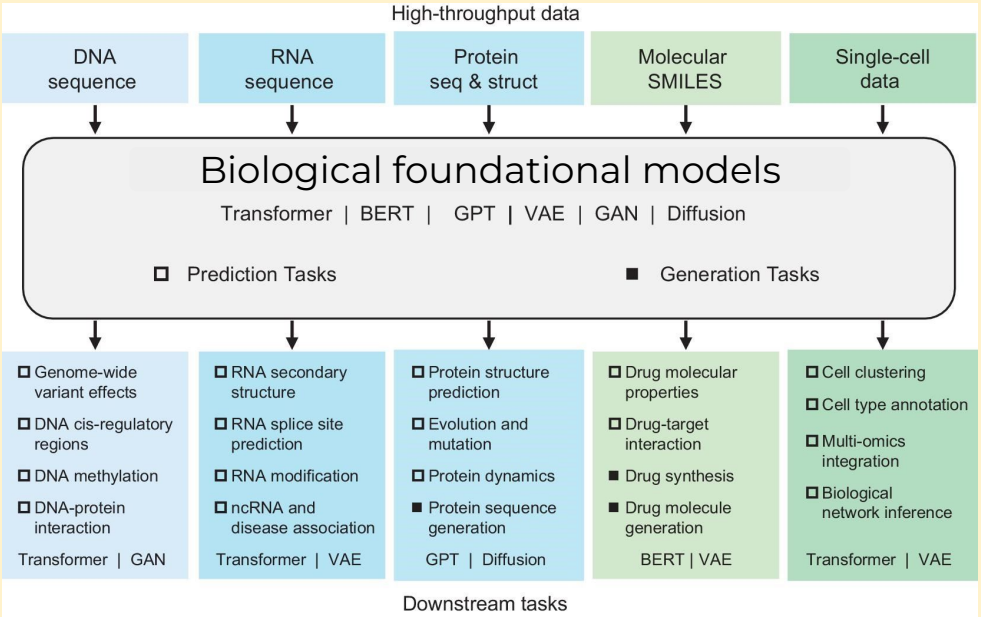
**Now**



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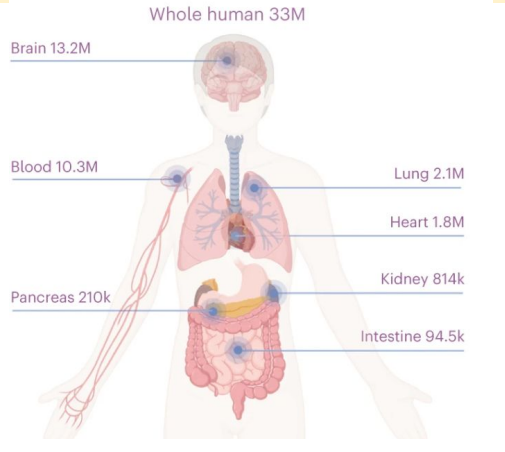
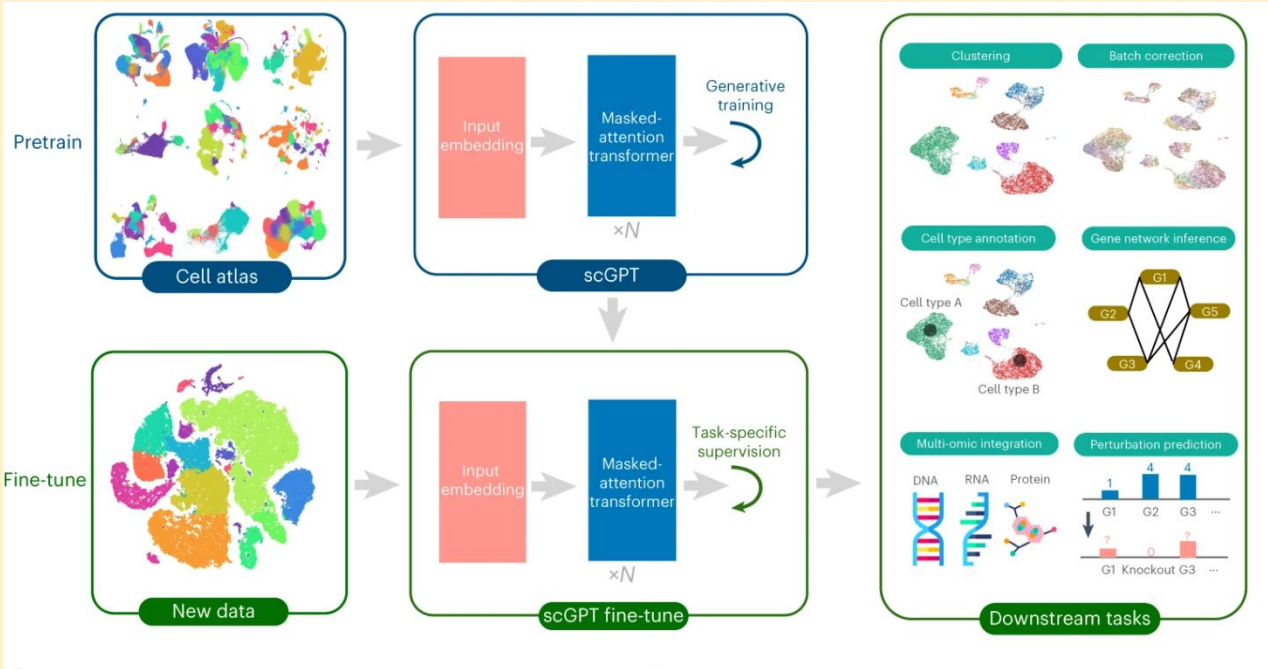
# Foundational models and LLMs

NLP
(Bio-LLMs)

## scGPT - Reading cell grammar

Trained with an **atlas** of **more** than **33M normal** cells






Cui, H., Wang, C., Maan, H. et al. scGPT: toward building a foundation model for single-cell multi-omics using generative AI. Nat Methods 21, 1470–1480 (2024). https://doi.org/10.1038/s41592-024-02201-0

# Foundational models and LLMs

NLP (Bio-LLMs)

## LLMs: beyond software

**DNA/RNA sequence analysis, functional prediction and structure prediction**

- HyenaDNA
- DNAGPT
- CombSAFE
- BERT-Enhancer
- DNABERT
- RoBERTa
- RNABERT
- GeoBoost2

**Protein sequence analysis, functional prediction and structure prediction**

- PTMGPT
- ProGen
- ESM
- ProtGPT
- EpiBERTope
- ELMo
- BepiPred-3.0
- TransPPMP
- ProteinBERT
- MSA Transformer
- BERT4Bitter

**Multi-Omics Data Analysis**

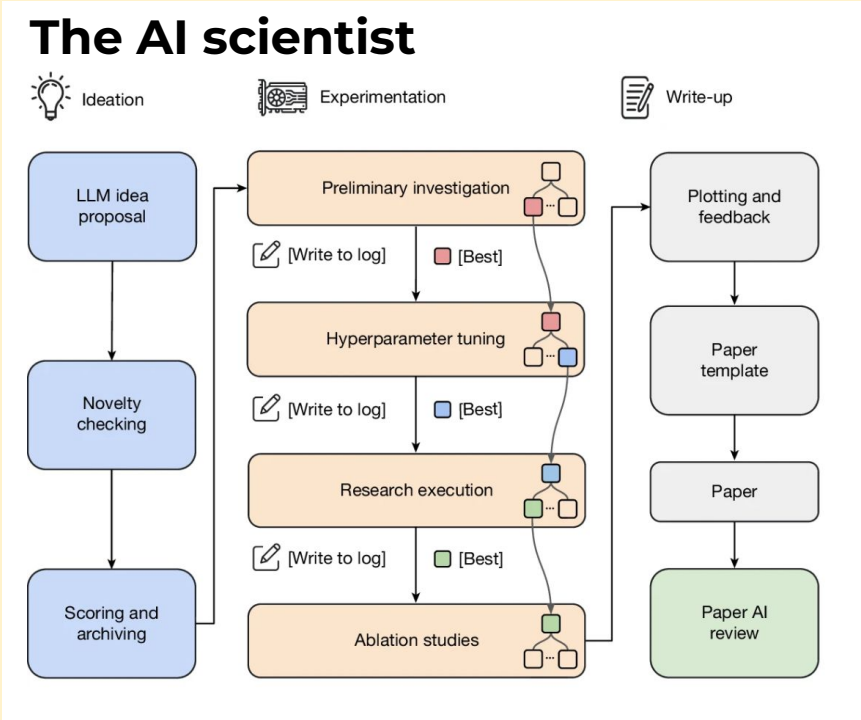
- BERT-TFBS
- scGPT
- GP-GPT
- pLM4Alg
- scELMo
- MuLan-Methyl
- iEnhancer-BERT
- scBERT
- TooT-PLM-ionCT
- UESolDS
- iDNA-ABT
- POOE
- mtx-COBRA
- DeepGene Transformer

**Computational Approaches in Drug Discovery and Design**

- MolGPT
- ChemBERTa
- SMILES-BERT
- PISTON
- MRCF
- K-BERT
- PharmBERT
- DTI-BERT
- TransDTI

**Biomedical Literature Mining**

- Galactica
- BioBERT
- ClinicalBERT
- GENEVIC
- MarkerGenie
- LBERT
- GenCLiP 3
- BioBERT




Lin A, *et al*. Bridging artificial intelligence and biological sciences: a comprehensive review of large language models in bioinformatics. Brief Bioinform. 2025 Jul 2;26(4):bbaf357. doi: 10.1093/bib/bbaf357.
Lu, C., Lu, C., Lange, R.T. et al. Towards end-to-end automation of AI research. Nature 651, 914–919 (2026). https://doi.org/10.1038/s41586-026-10265-5

# AI in drug discovery

Digital Chemistry

## From a Tortuous Path to a Streamlined Pipeline


### Target structure prediction

**AlphaFold**: Predicted 3D structure >200M proteins

### Virtual screening

ML models screens billions of compounds in silico, reducing wet lab screening

### Generative chemistry

Models in silico generate novel drug-like molecules with desired properties

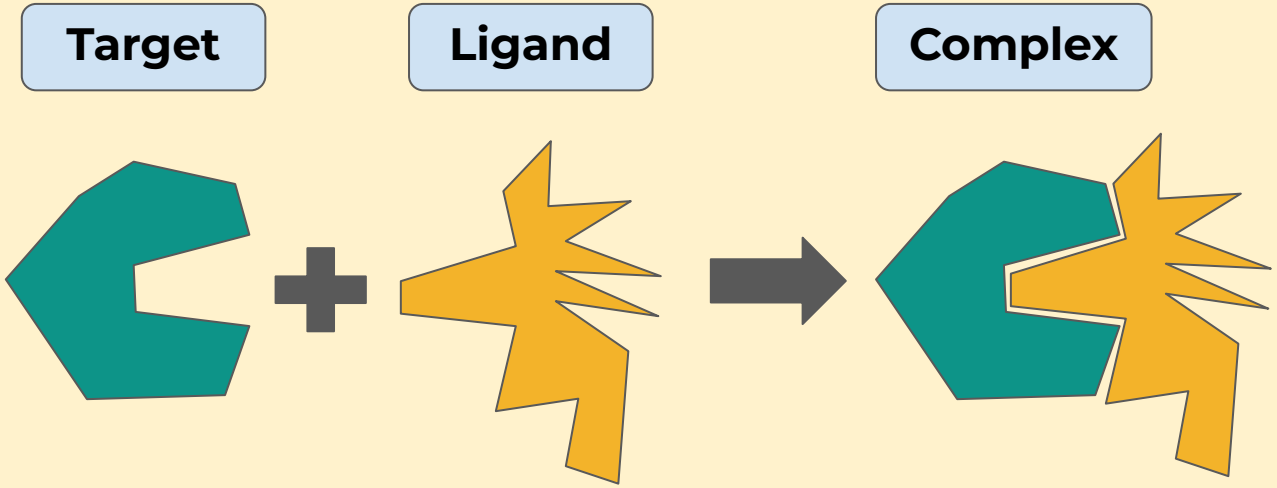
### ADMET prediction

AI predicts absorption, distribution, metabolism, excretion and toxicity early

# DiffDock: difussion and GNNs

Digital Chemistry

## Generative AI for molecular docking

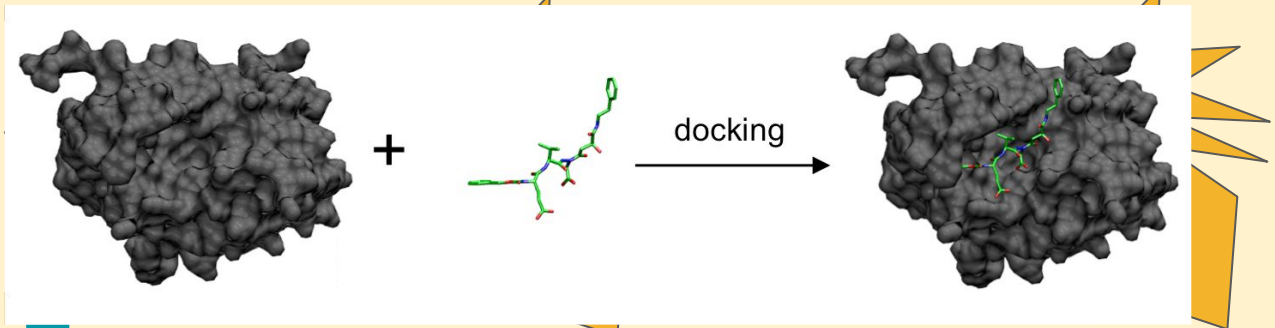


# DiffDock: difussion and GNNs

Digital Chemistry

## Generative AI for molecular docking

**Target** + **Ligand** → **Complex**




**Traditional**

**Brute force search**: **Test thousands** of **random** rotations and positions **until** an **energy minimum** is **found** (minutes to hours)

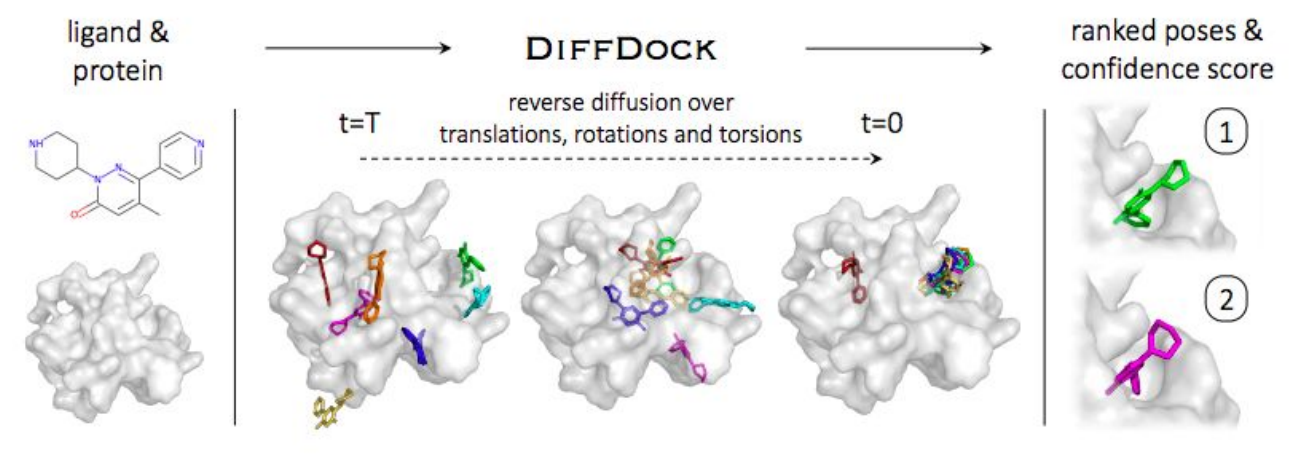
Estimating this binding site is a **computationally intensive search problem**.

# DiffDock: difussion and GNNs

Digital Chemistry

## Generative AI for molecular docking

**Initial noise** → **Reverse diffusion** → **Final pose**




**DiffDock**

**Diffusion models** to 'learn' the optimal position, achieving **unprecedented accuracy** in a matter of seconds.

# Challenges & Ethical considerations

**Data quality & bias**

Models trained on biased data can perpetuate health disparities.

**Interpretability (XAI)**

Black box models hinder clinical trust. Explainable AI techniques are essential.

**Regulatory approval**

FDA, EMA frameworks for AI as software as a Medical device (SaMD) are still evolving rapidly.

**Data privacy**

Patient data governance, federated learning, and differential privacy are critical for compliant AI development.

**Reproducibility**

Many published AI models lack code/data sharing - reproducibility crisis mirrors classical biomedical research.

**Clinical validation**

Prospective clinical trials needed to prove real-world impact beyond in silico tests.

# The road ahead

| | |
|---|---|
| **Now** | AI-assisted imaging, genomics,<br>drug screening validated tools in research pipelines |
| **2026-28** | AI co-pilots in clinical settings<br>FDA/EMA-approved AI diagnostics mainstream |
| **2029-32** | Multimodal foundation models integrating imaging +<br>omics + EHR for holistic patient modeling |
| **2033+** | Autonomous AI-driven hypothesis generation and<br>experimental design closing the R&D loop |

**The question is no longer IF AI will transform biomedicine, but HOW FAST and with what safeguards.**

# Take home message

a. AI is not a single tool, it's a **family of techniques** each **suited** to **different biomedical problems**.

b. **Proven impact areas**: protein structure prediction, medical imaging, drug virtual screening.

c. **Challenges remain**: data bias, interpretability, regulatory pathways, and rigorous clinical validation.

d. Biomedical **researchers benefit from AI literacy**, not necessarily coding expertise, but conceptual understanding.

Thanks!

# ANY QUESTIONS?

You can also find me at:

aberralgonzalez@usal.es

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