生命科学研究における AI 活用の動向、展望、課題

医薬基盤・健康・栄養研究所
徳島大学 先端酵素学研究所

夏目やよい

DEVELOPERS OF ALPHAFOLD WIN CHEMISTRY NOBEL

The prize celebrates artificial-intelligence tools that could revolutionize drug discovery.

By Ewen Callaway

For the first time – but probably not the last – a scientific breakthrough enabled by artificial intelligence (AI) has been recognized with a Nobel prize. The 2024 chemistry Nobel was awarded to John Jumper and Demis Hassabis at Google DeepMind in London, for developing a game-changing AI tool called AlphaFold for predicting protein structures, and David Baker, at the University of Washington in Seattle, for his work on computational protein design, which has been bolstered by AI in the past few years.

"I hope when we look back on AlphaFold, it will be the first proof point of AI's incredible potential to accelerate scientific discovery," Hassabis said at a press briefing at DeepMind on 9 October. "It's so unreal at this moment."

The impact of AlphaFold, which was unveiled just a few years ago, has been nothing short of transformative. The tool has made protein structures – often highly accurate ones – available to researchers at the touch of a button, and has enabled experiments that were unimaginable a decade ago. "It's a major revolution," says Christine Orengo, a computational biologist at University College London, whose laboratory has used AlphaFold-predicted structures to uncover new proteins.

"It has long been a dream to learn to predict the three-dimensional structure of proteins from knowing their amino-acid sequences. For several decades, this was considered impossible," said Nobel committee chair Heiner Linke, who researches nanoscience at Lund University in Sweden, during the prize announcement on 9 October. This year's laureates "have cracked the code", he added.

DeepMind debuted AlphaFold in 2018, when it won a biennial protein-structure prediction

David Baker, Demis Hassabis and John Jumper (left to right) won the 2024 chemistry Nobel.

Nature | Vol 634 | 17 October 2024 | **525**

2024年は、AIが科学にもたらした
ブレイクスルーに改めて
注目が集まった年でした

タンパク質の構造を設計するAI
David Baker

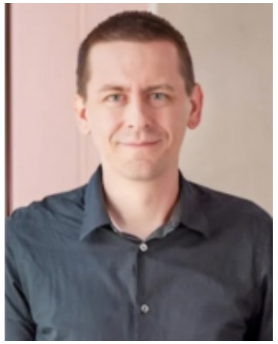
タンパク質の構造を予測するAI
「AlphaFold」
Demis Hassabis、John Jumper

33rd CONFERENCE ON
Intelligent Systems for Molecular Biology

AND THE 24th
European Conference on Computational Biology

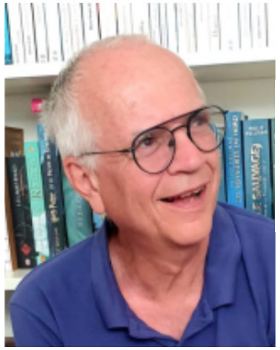
DATES: July 20 – 24

Distinguished Keynotes



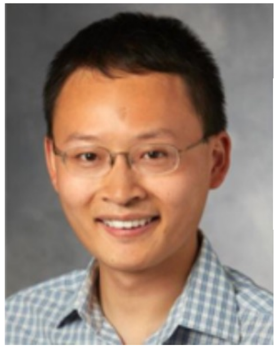
John Jumper
Google DeepMind
United Kingdom

AlphaFold



Amos Bairoch
SIB Swiss Institute of Bioinformatics
Switzerland

Swiss-Prot



James Zou
Stanford University
United States

Agentic AI

Charlotte Deane
University of Oxford
United Kingdom

Complex interaction

David Baker
University of Washington
United States

AlphaFold

Fabian Theis
Helmholtz Munich
Germany

Human Cell Atlas

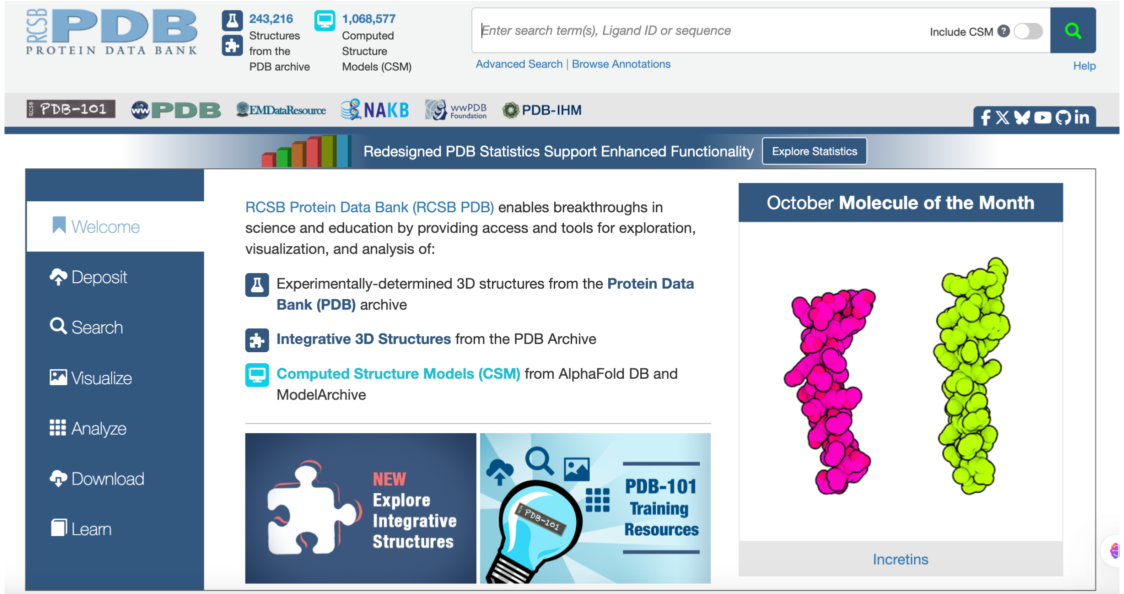
https://www.iscb.org/ismbeccb2025/programme-agenda/distinguished-keynotes

Driven by data

Hassabis, DeepMind's co-founder and chief executive, and Jumper, head of the AlphaFold team, led the development of AlphaFold2. To predict protein structures, the neural network incorporates data from libraries of hundreds of thousands of structures and millions of sequences from related proteins – all of which hold information about their shapes.

AlphaFold's success is due in no small part to the Protein Data Bank, a freely available repository of more than 200,000 protein structures determined using methods including X-ray crystallography and cryo-electron microscopy. "It's humbling every time we train [AlphaFold] on years of effort. Each data point is years of effort from someone," Jumper said at the DeepMind press briefing.

Nature (2024-10-09) | DOI: 10.1038/d41586-024-03214-7



Redesigned PDB Statistics Support Enhanced Functionality

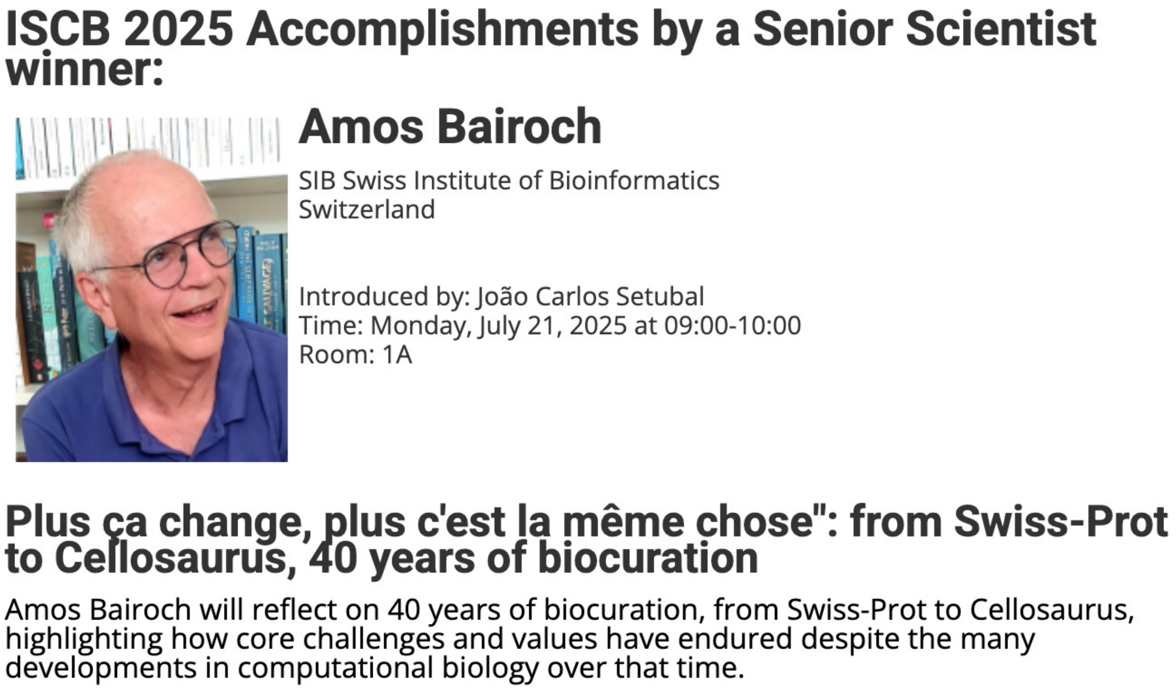
RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

- Experimentally-determined 3D structures from the **Protein Data Bank (PDB)** archive
- **Integrative 3D Structures** from the PDB Archive
- **Computed Structure Models (CSM)** from AlphaFold DB and ModelArchive

October **Molecule of the Month**

https://www.rcsb.org/

「何年も努力してAlphaFoldを訓練するたびに
謙虚な気持ちになる。
それぞれのデータポイントは、
誰かの何年もの努力の結晶だから。」



ISCB 2025 Accomplishments by a Senior Scientist winner:

Amos Bairoch

SIB Swiss Institute of Bioinformatics
Switzerland

Introduced by: João Carlos Setubal
Time: Monday, July 21, 2025 at 09:00-10:00
Room: 1A

Plus ça change, plus c'est la même chose": from Swiss-Prot to Cellosaurus, 40 years of biocuration

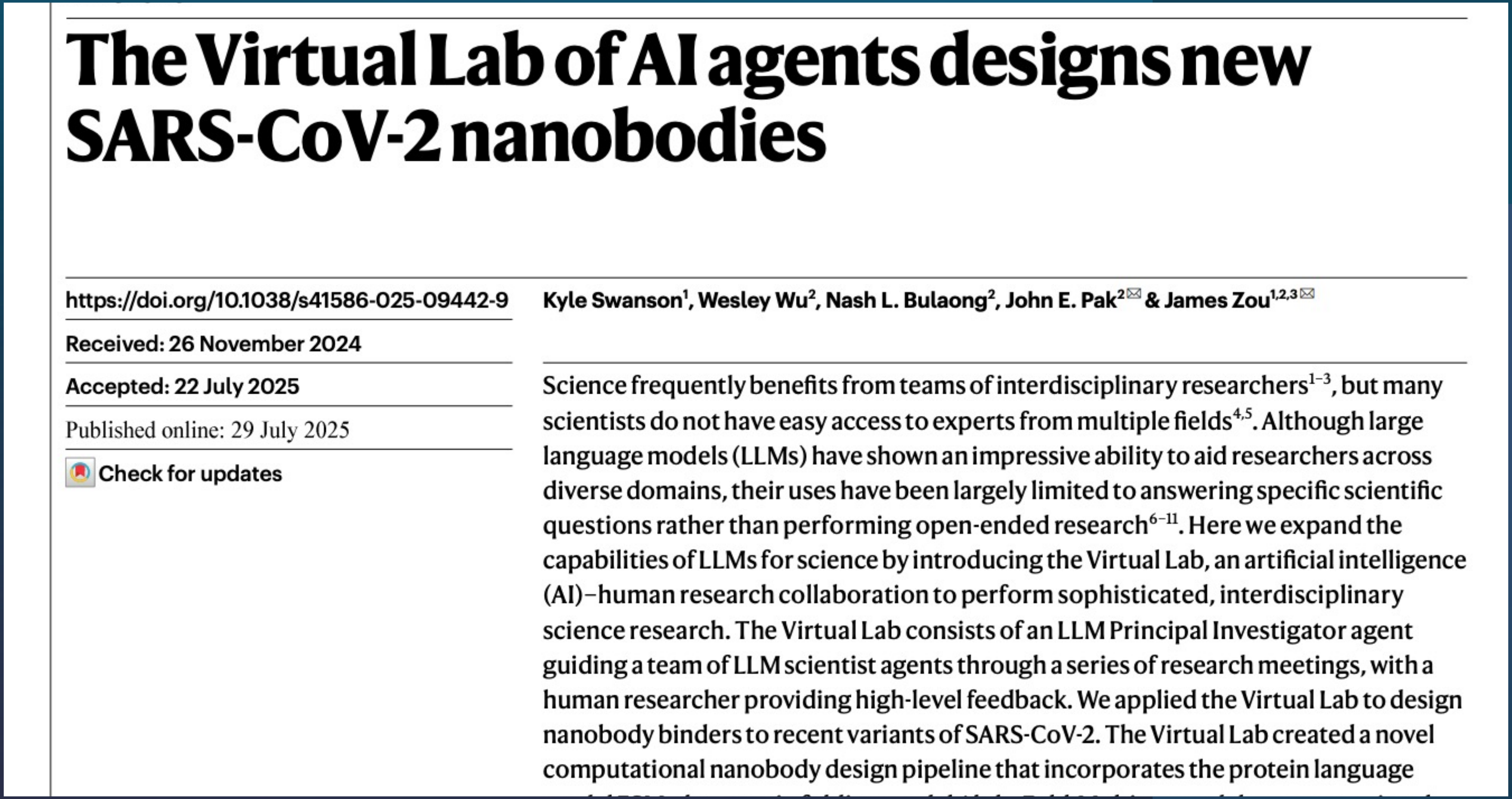
Amos Bairoch will reflect on 40 years of biocuration, from Swiss-Prot to Cellosaurus, highlighting how core challenges and values have endured despite the many developments in computational biology over that time.

- バイオキュレーションに対する
  資金不足、過小評価
  「自動化で代替できる」？

- 専門的知識と人手によるキュレーションは
  不可欠な科学基盤である

- バイオキュレーションの価値を
  正当に評価・支援する仕組みが必要

https://www.iscb.org/ismbeccb2025/programme-agenda/distinguished-keynotes



The Virtual Lab of AI agents designs new SARS-CoV-2 nanobodies

https://doi.org/10.1038/s41586-025-09442-9

Received: 26 November 2024

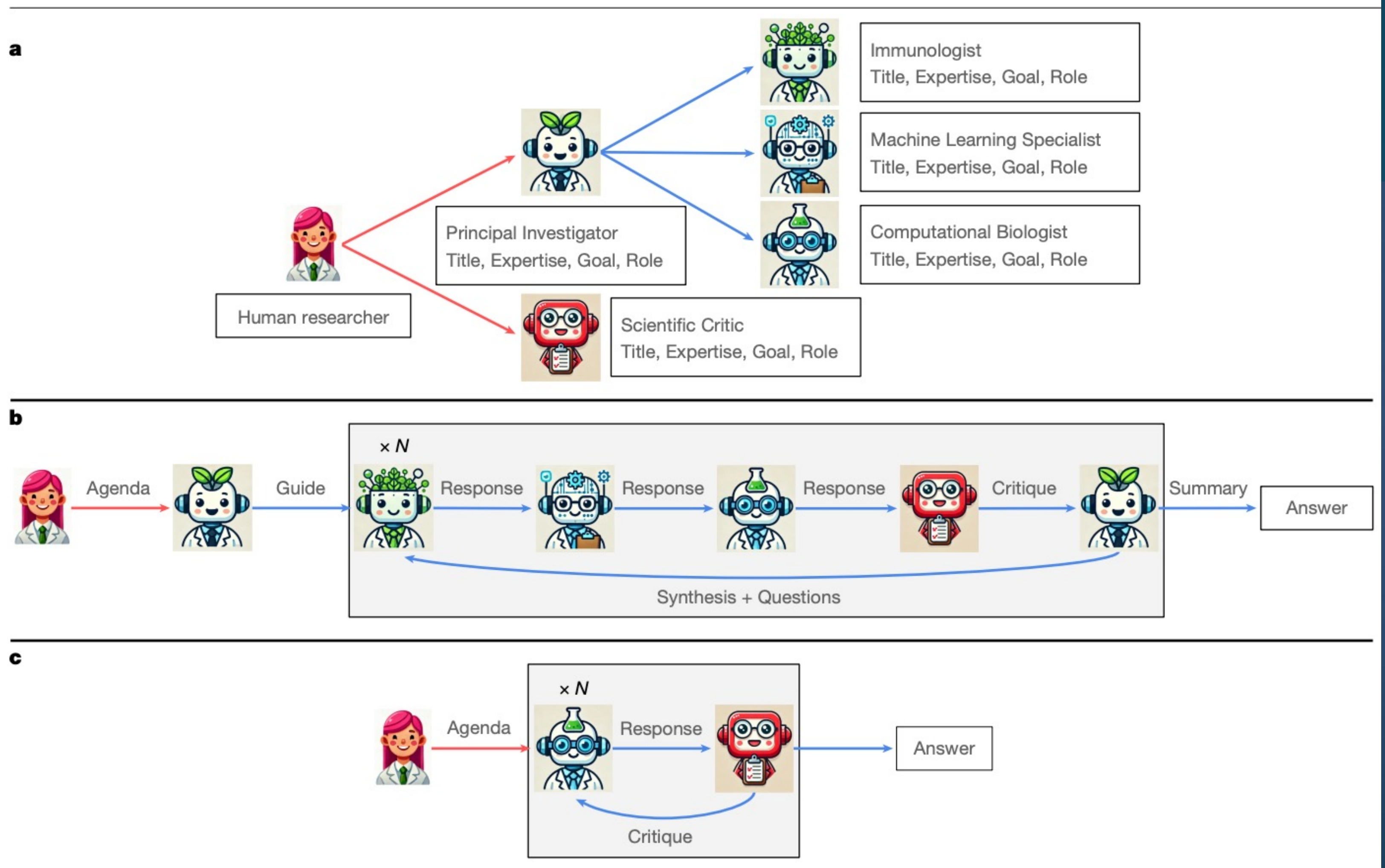
Accepted: 22 July 2025

Kyle Swanson[1], Wesley Wu[2], Nash L. Bulaong[2], John E. Pak[2]✉ & James Zou[1,2,3]✉

Science frequently benefits from teams of interdisciplinary researchers[1–3], but many scientists do not have easy access to experts from multiple fields[4,5]. Although large language models (LLMs) have shown an impressive ability to aid researchers across diverse domains, their uses have been largely limited to answering specific scientific questions rather than performing open-ended research[6–11]. Here we expand the capabilities of LLMs for science by introducing the Virtual Lab, an artificial intelligence (AI)–human research collaboration to perform sophisticated, interdisciplinary science research. The Virtual Lab consists of an LLM Principal Investigator agent guiding a team of LLM scientist agents through a series of research meetings, with a human researcher providing high-level feedback. We applied the Virtual Lab to design nanobody binders to recent variants of SARS-CoV-2. The Virtual Lab created a novel computational nanobody design pipeline that incorporates the protein language

Nature (2025). https://doi.org/10.1038/s41586-025-09442-9

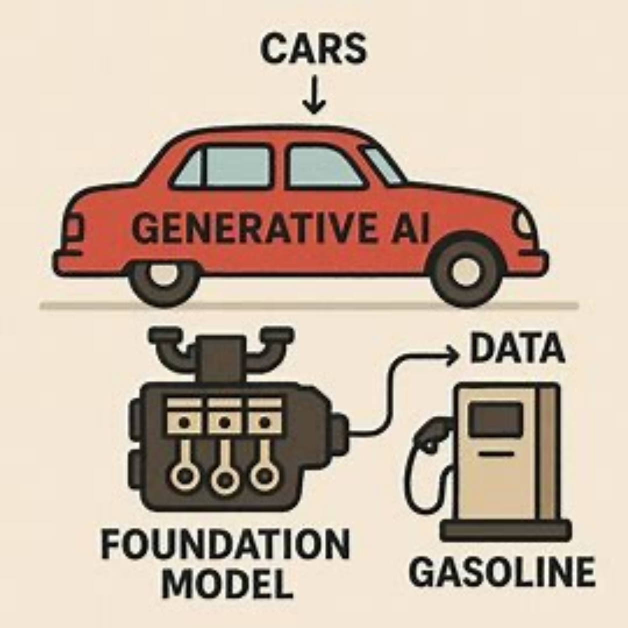
The Virtual Lab of AI agents designs new SARS-CoV-2 nanobodies



Nature (2025). https://doi.org/10.1038/s41586-025-09442-9

生命科学分野の多様なデータ（言語、画像、配列、構造など）を学習して
構築される基盤モデルと、それを活用した生成AIの開発・利活用

AIによる生成→実験による検証→再学習　のループによる研究の加速



Microsoft Bing Image Creatorにより作成

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技術よりも高品質データの確保がボトルネック？