



The Science of Acceleration: What Makes Change Happen Faster?

March 27 2025

Our Core Values



Our core values are the principles we embody daily, shaping our work, collaborations, and contributions. They form the essence of Quantori's culture and serve as the compass that guides us on our journey, making a positive impact on the industry and the world we operate in.

Integrity

Guided by Principles, Driven by Purpose

Integrity is the foundation of trust, fostering strong relationships with our partners, clients, and team members.



Dignity

Where Respect Meets Progress

We believe everyone should receive dignified and respectful treatment, nurturing an inclusive and supportive work environment.



Empathy

Building Solutions That Begin with Understanding

Empathy fuels collaboration, enabling us to forge deeper connections and cultivate a workplace characterized by compassion and understanding.



Accountability

Driving Progress, Delivering Results

Accountability ensures the fulfillment of our commitments, with reflections and learnings from challenges faced and driving continuous improvement.



Innovation

Innovating Today for a Better Tomorrow

Innovation fuels our growth, enabling us to pioneer solutions that have a significant impact on the life sciences, healthcare, and pharma industries.



Webinar Speakers



Anna Ivanova

Sr. Bioinformatician & BigData Engineer

The Importance of Scientific Communications



Maria Selifanova

Bioinformatician

From Mechanisms to Systems:
Can Biologists Fix the Ratio?



Karina Pats

ML Engineer

Deep Learning: a Powerful Tool for Solving Mysteries of Life Science

The Importance of Scientific Communications

The background features a series of overlapping, curved shapes in various shades of blue and yellow. The shapes are soft-edged and create a dynamic, layered effect. The colors transition from a deep blue on the left to a bright yellow on the right, with intermediate shades of teal and light blue.

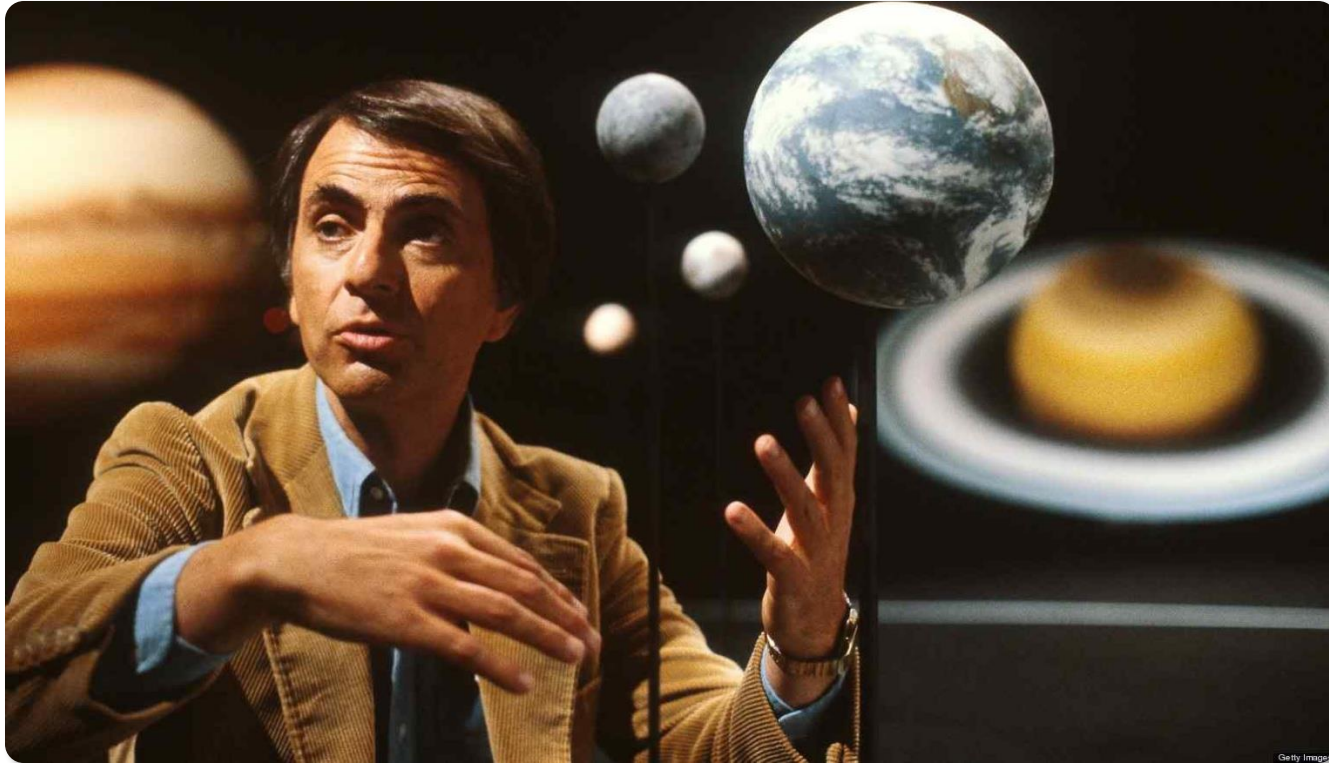
Background



The Adventures of a Small Yellow Submarine

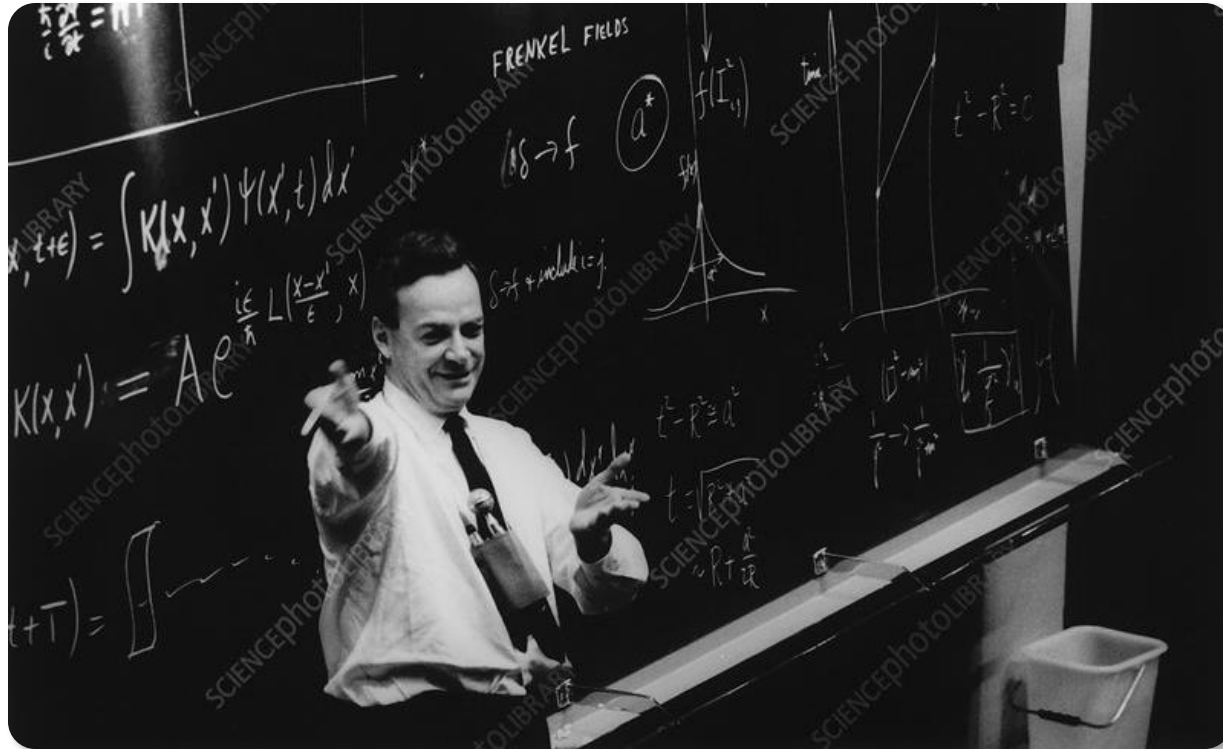


The “Sagan Effect”



Cosmos: A Personal Voyage • 1980 • 13 episodes

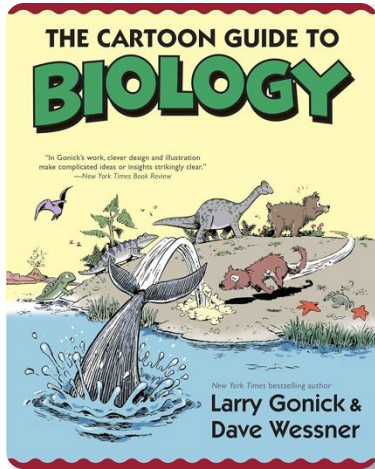
“You can’t be a good scientist and a showman at the same time.”



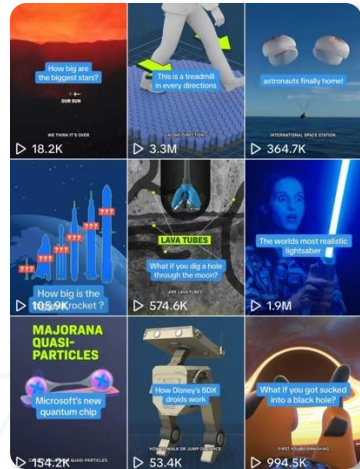
Credit [CERN / SCIENCE PHOTO LIBRARY](#)

Judged Science Communication Formats

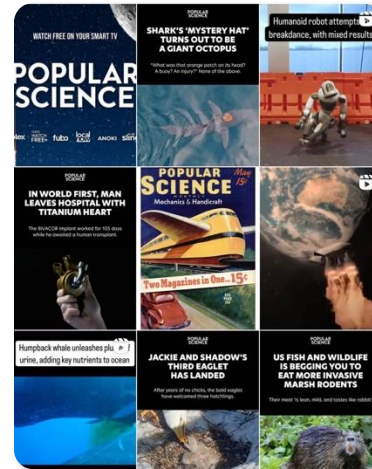
Comics



TikToks



Instagram Posts

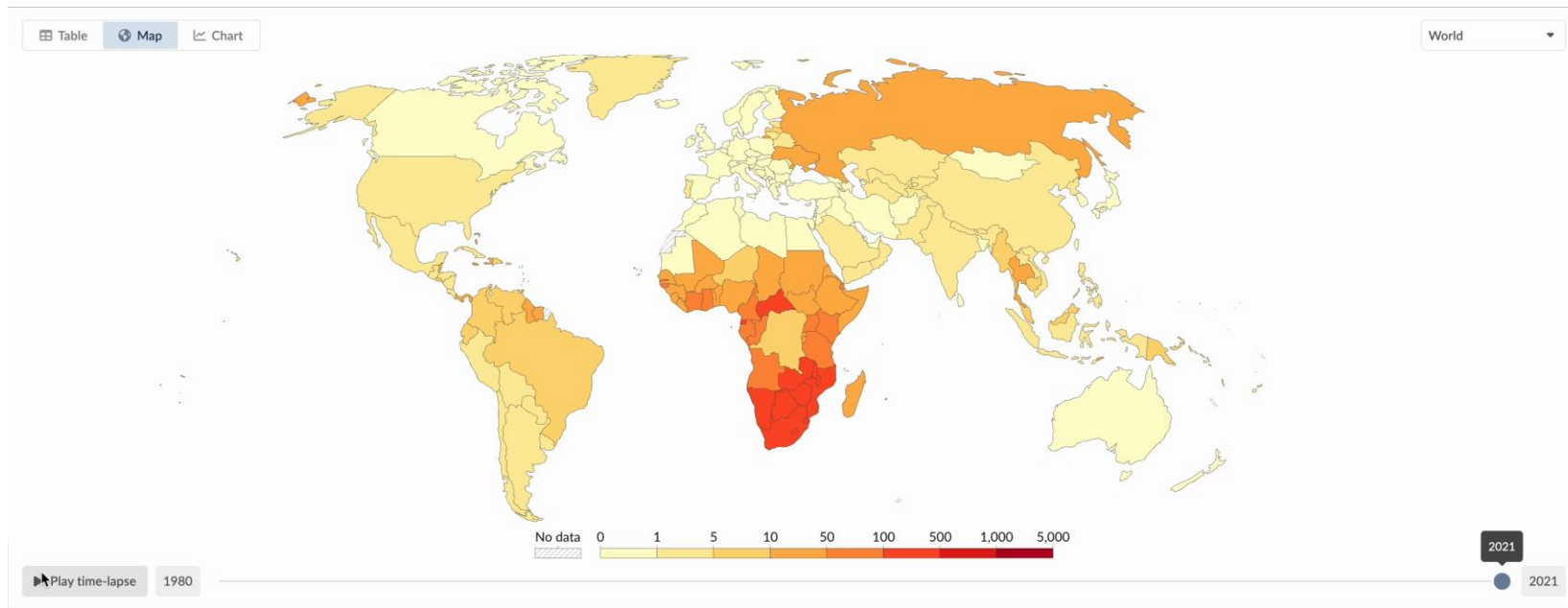


X (Twitter)



Death Rate from HIV/AIDS

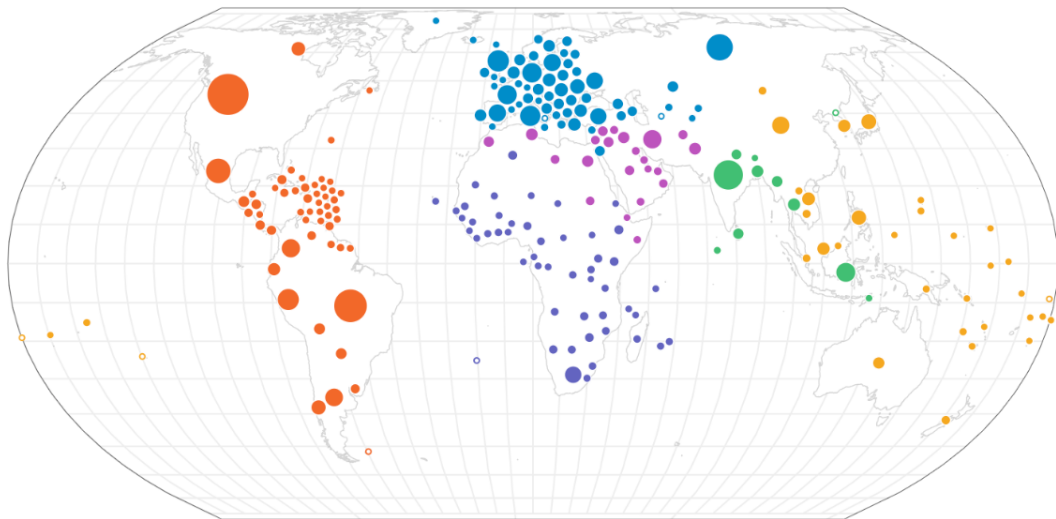
The number of deaths from HIV/AIDS per 100,000 people.



Data source: IHME, Global Burden of Disease (2024)

Number of COVID-19 deaths reported to WHO (cumulative total)

World



7,090,480 **+469**
increase on previous 7 days

Reported COVID-19 deaths

World, 7 days to 9 March 2025

Number of COVID-19 deaths reported to WHO (cumulative total)

World

Country	Deaths ▾
World	7.1m
United States of America	1.2m
Brazil	702k
Show 229 more	
Saint Helena	0

Source: <https://data.who.int/dashboards/covid19/deaths>

Podcasts Recommendations

This Podcast Will Kill You



Radiolab



NASA podcasts



Questions



Anna Ivanova

Sr. Bioinformatician & BigData Engineer

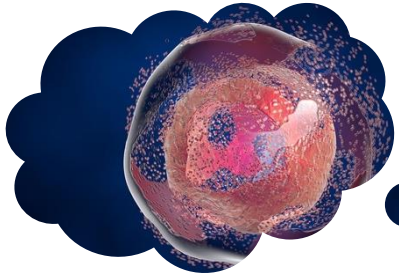
Instagram: [Lab.Mouse](#)

LinkedIN: [Anna Ivanova](#)



**From Mechanisms to Systems:
Can Biologists Fix the Ratio?**

David's Model: Cycle of Biological Research



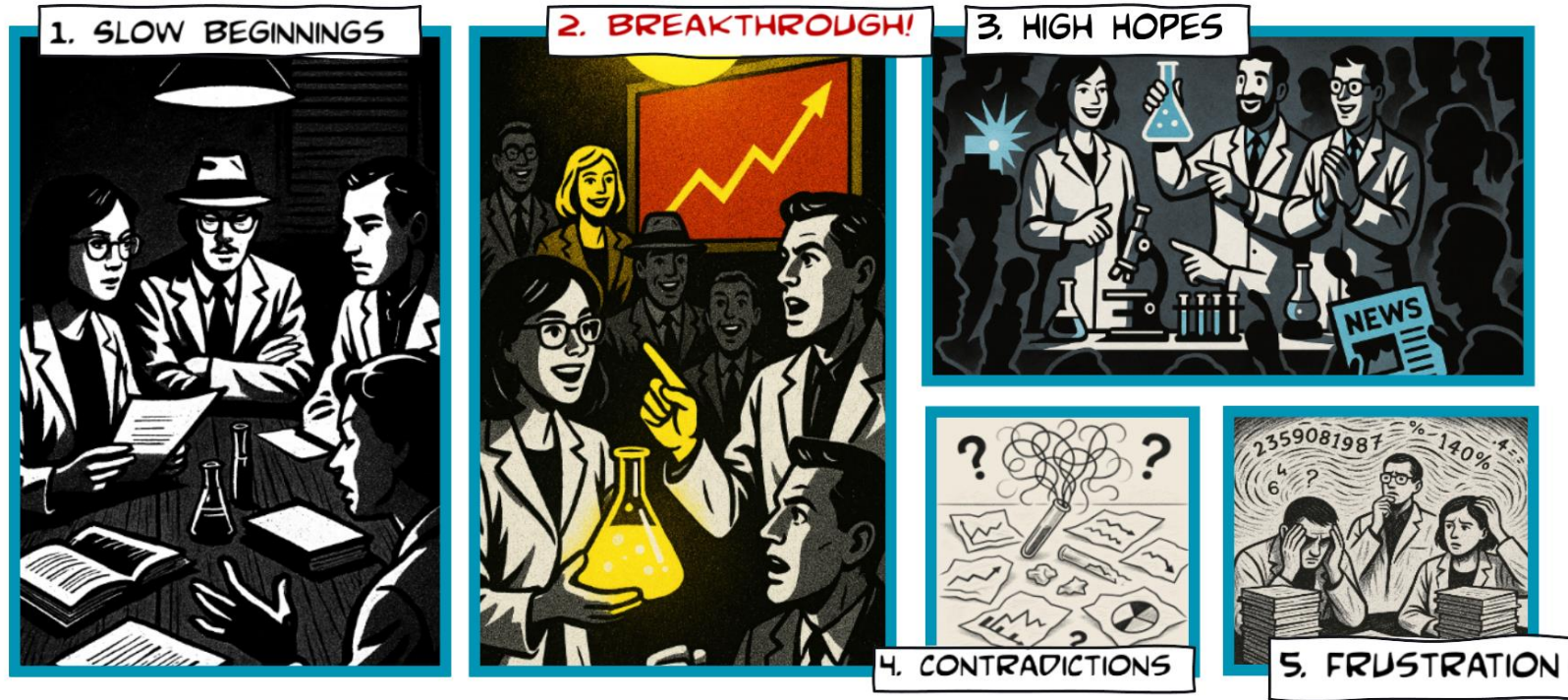
Yuri Lazebnik



David S. Papermaster



David's Model: Cycle of Biological Research

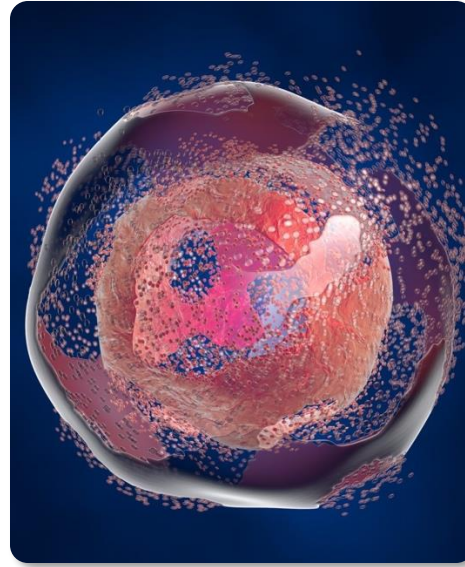


“Can a biologist fix a radio? – Or, what I learned while studying apoptosis”

Yuri Lazebnik



Programmed Cell Death



Broken Transistor Radio

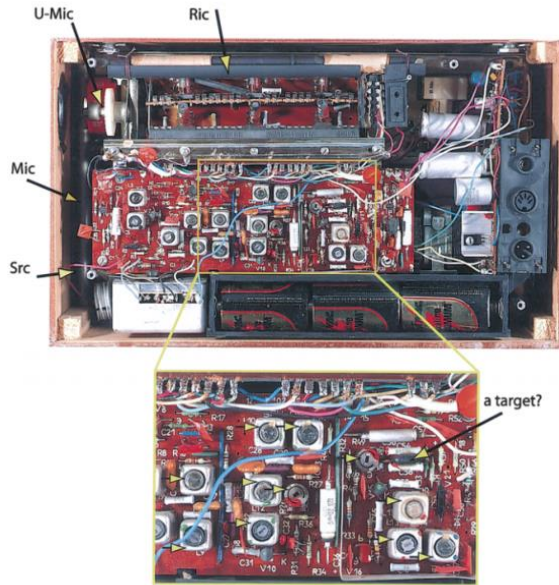


Figure 1. The radio that has been used in this study

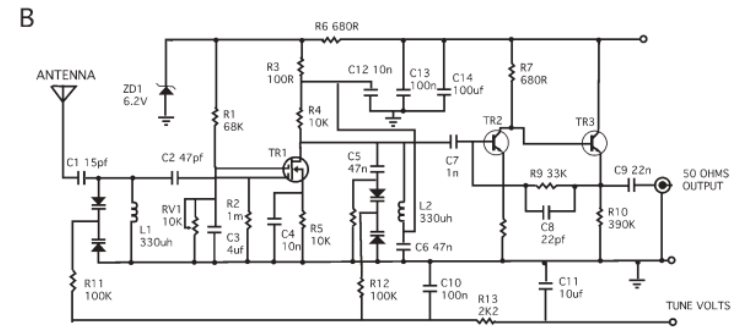
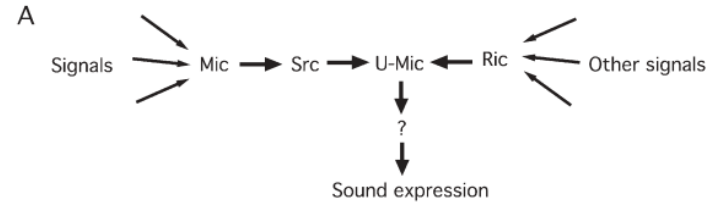
Lazebnik, Yuri. "Can a biologist fix a radio?—Or, what I learned while studying apoptosis." *Cancer cell* 2.3 (2002): 179-182.

Lazebnik's Thought Experiment

The insides of the radio



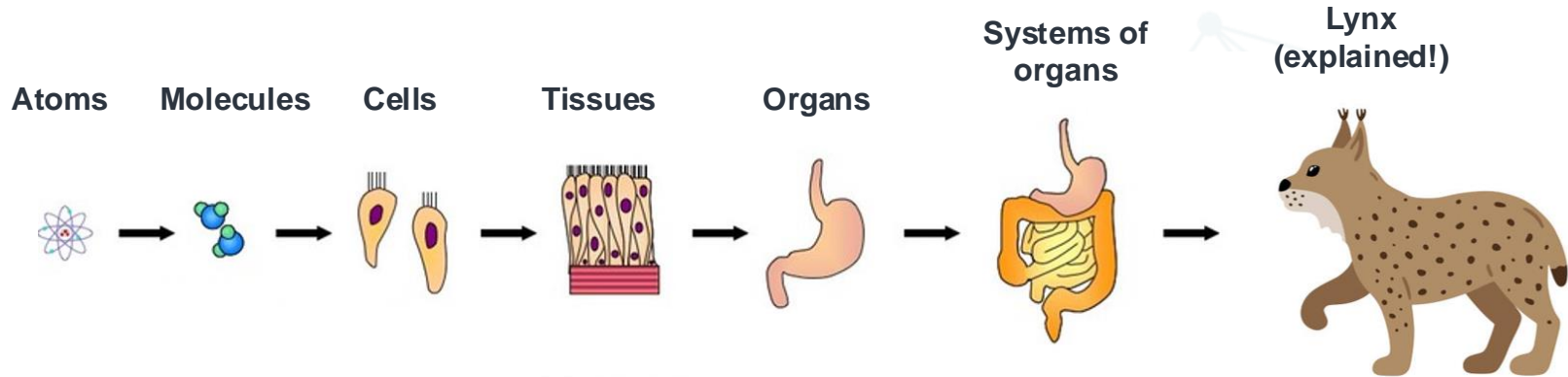
Biologists' (A) vs engineers' (B) process schemas



Lazebnik, Yuri. "Can a biologist fix a radio?—Or, what I learned while studying apoptosis." *Cancer cell* 2.3 (2002): 179-182.

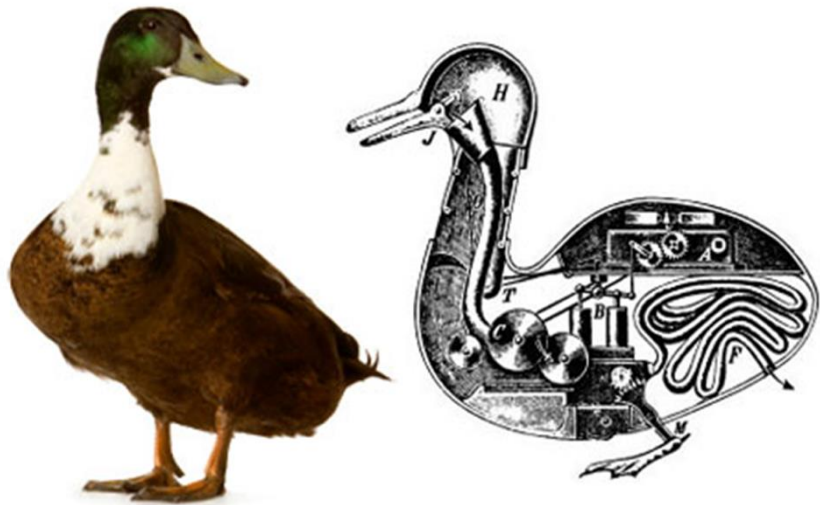
Reductionism

is a methodological perspective that **complex systems can be fully understood by breaking them down into their constituent parts**, studying and analyzing these components in isolation, without necessarily reconciling them back into the whole.



Dupré, John. *Processes of life: Essays in the philosophy of biology*. Oxford University Press, 2012.

Duck Reductionism



“

Duck behaviour is the sum of its automatically behaving parts.

Descartes, 1662

Descartes, René. *De homine*. Vol. 6. Hack, 1969.

Reductionism: Triumph of Molecular Biology

Rosalind Franklin, 1955



James Watson and Francis Crick, 1953



Watson & Crick (1953) proposed the **DNA double-helix model** based on Rosalind Franklin's X-ray diffraction data, showing how base pairing encodes genetic information.

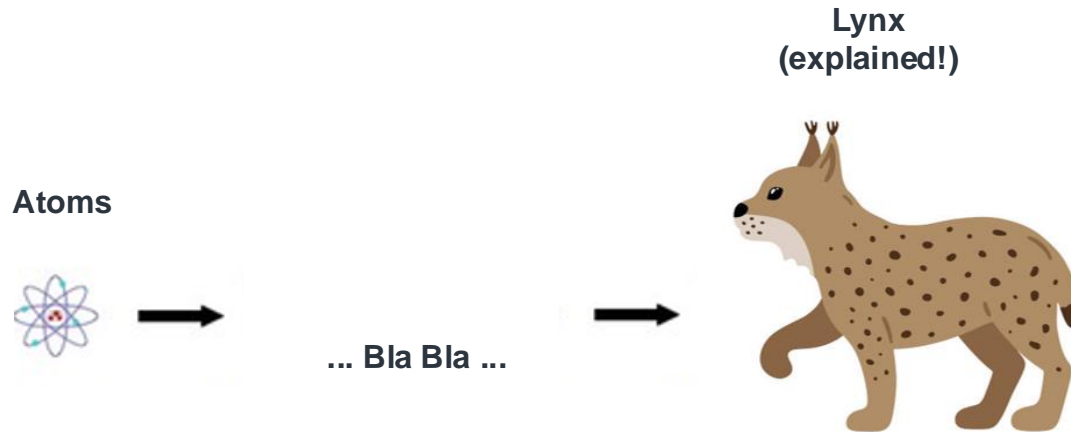
Watson, James D., and Francis HC Crick. "The structure of DNA." *Cold Spring Harbor symposia on quantitative biology*. Vol. 18. Cold Spring Harbor Laboratory Press, 1953.

Reductionism: Triumph of Molecular Biology

- 1953 – Double helix (Watson & Crick) — identified DNA as the hereditary molecule
- 1958 – First protein structure (Kendrew & Perutz) — revealed 3D link between sequence and function
- 1958 – Central Dogma (Crick) — defined information flow: DNA → RNA → protein
- 1961 – Genetic code (Nirenberg & Matthaei) — showed codons specify amino acids
- 1961 – Lac operon (Jacob & Monod) — demonstrated protein–DNA control of gene expression
- 1961 – Cell-free translation (Nirenberg) — produced proteins from purified components
- 1972 – Recombinant DNA (Cohen & Boyer) — enabled gene isolation and cloning
- 1977 – DNA sequencing (Sanger) — first method to read nucleotide sequences
- 1962 – Viral capsid self-assembly (Caspar & Klug) — proteins spontaneously form functional shell
- 2003 – Human Genome Project — delivered the complete human DNA blueprint
- 2012 – CRISPR-Cas (Doudna & Charpentier) — established precise genome editing tool
- **... and much more**

Physicalism

Is an idea that every **biological explanation** could be reduced by **explanations in chemistry and physics**.



Dupré, John. *Processes of life: Essays in the philosophy of biology*. Oxford University Press, 2012.

Emergent Properties

– are unexpected properties that **arise when combining** individual components within a system.



Emergence

Interactions
networks

Processual
(dynamic)
nature

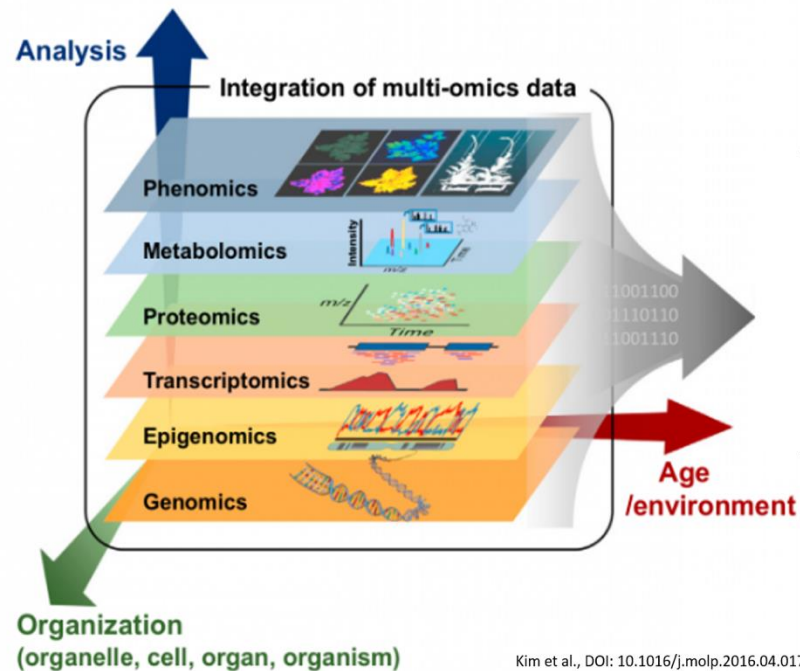
Multi-level
organization

Feedback
&
regulation

Context-dependence and
relational properties

Søren Solkær Black Sun #102 Rome Italy 2022 Archival pigment print on 325gsm Hahnemüle Baryta paper © Søren Solkær

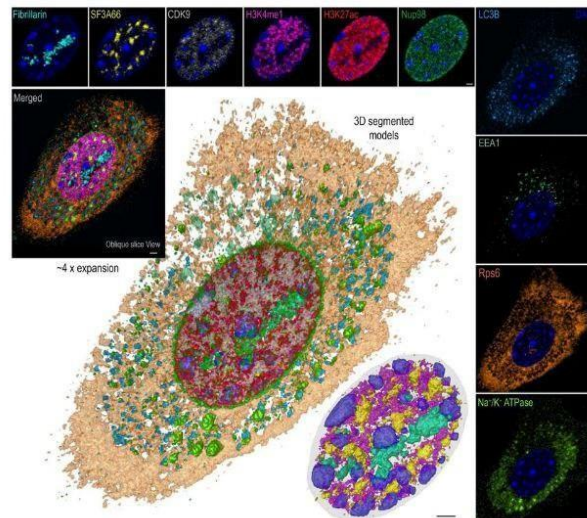
Mutiomics Data Integration



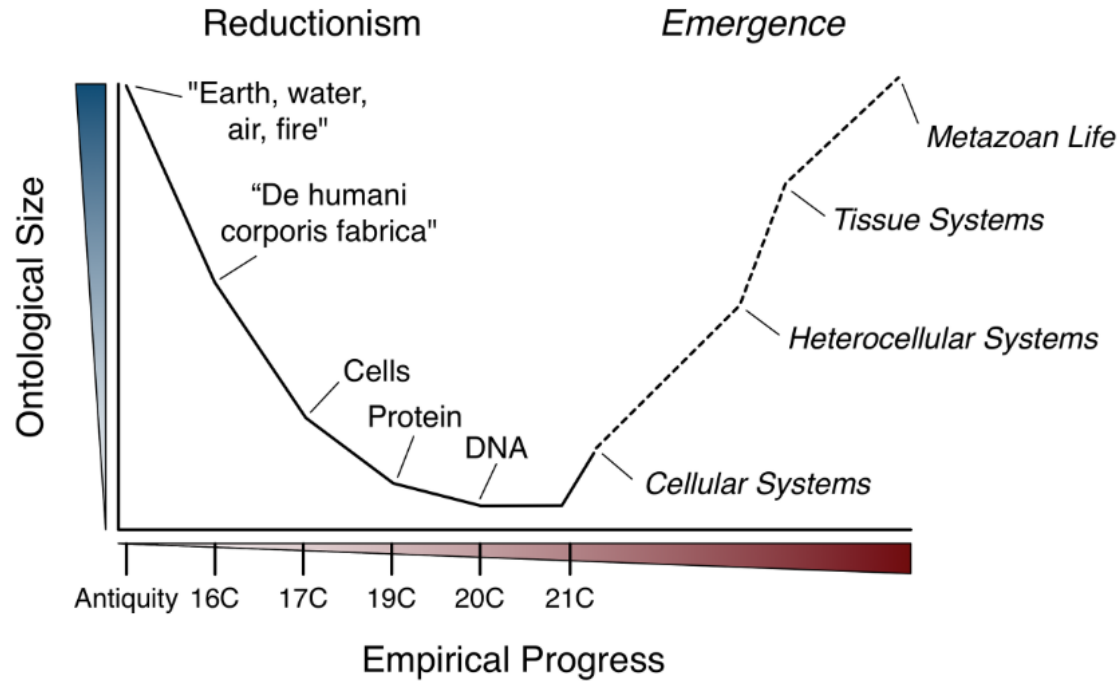
Spatial Mutiomics

Deep-tissue transcriptomics and subcellular imaging at high spatial resolution

Valentina Gandini[†], Jun Kim[†], Liang-Zhong Yang, Yumin Lian, Takashi Kawase, Amy Hu, Konrad Rokicki, Greg Fleishman, Paul Tillberg, Alejandro Aguilera Castrejon, Carsen Stringer, Stephan Preibisch, Zhe J. Liu*

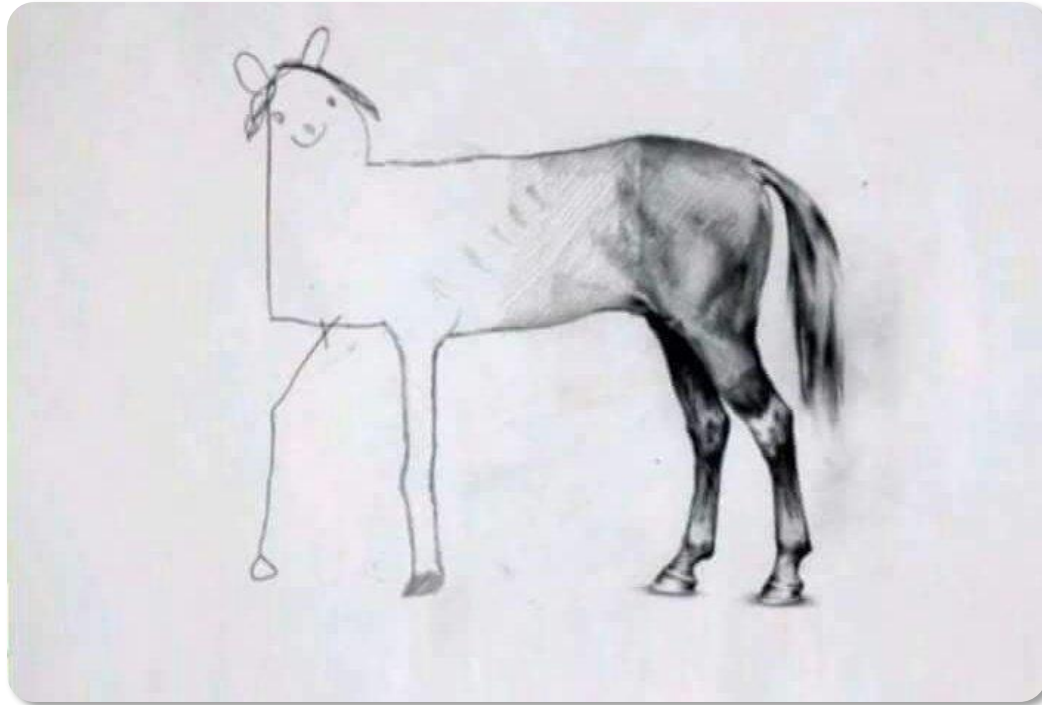


Reductionist Valley

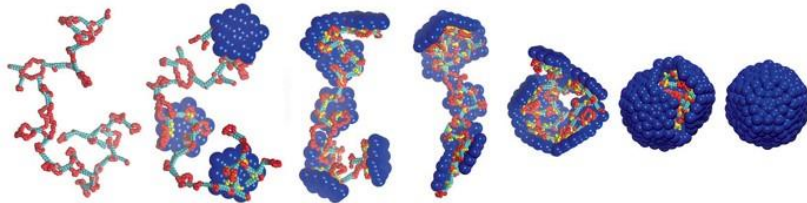


<https://tape-lab.com/blog/2016/8/25/escape-from-reductionist-valley>

How to Find a Balance?



DNA is the Blueprint of Life ... or Is It?

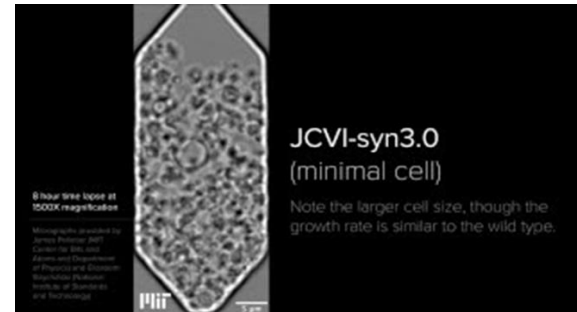


Reductionist thesis:

“DNA alone encodes all the information needed to build and run a living system.”

Example: In cell-free systems, DNA alone directs protein production, and viral coat proteins can spontaneously assemble into a complete shell.

Fraenkel-Conrat, Heinz, and Robley C. Williams. "Reconstitution of active tobacco mosaic virus from its inactive protein and nucleic acid components."(1955)



Holistic thesis:

“Hereditary information resides not just in DNA but in the entire genome–cell machinery system.”

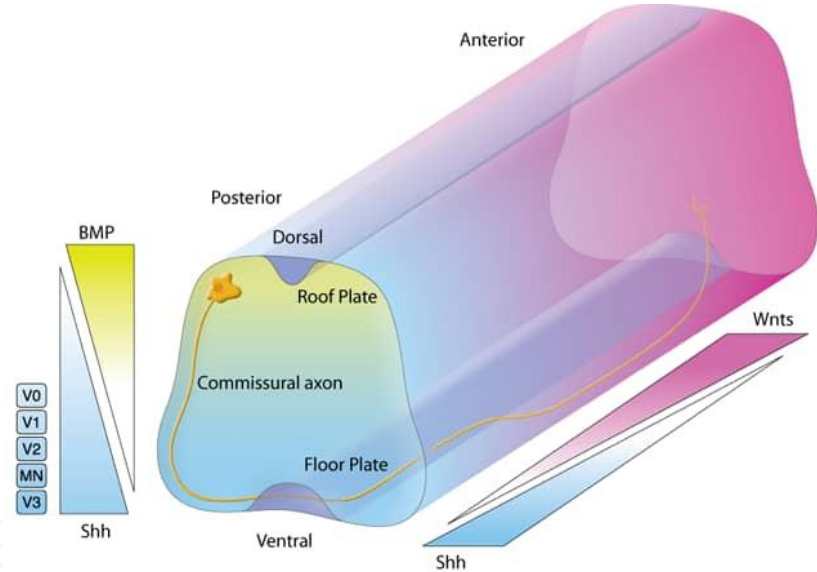
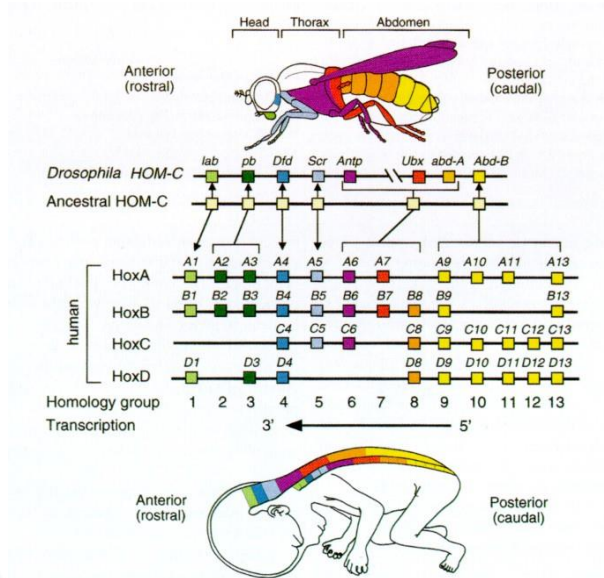
Example: Even the JCVI syn3.0 minimal genome can't build a cell from DNA alone—it still needs existing ribosomes, membranes, and enzymes.

Hutchison III, Clyde A., et al. "Design and synthesis of a minimal bacterial genome." *Science* 351.6280 (2016): aad6253.

Direction of Causation: Embryonic Development

Reductionist, upward causation,
Hox genes

Holistic, downward causation,
morphogens gradient



© R&D Systems, Inc.

Mark, Manuel, Filippo M. Rijli, and Pierre Chambon. "Homeobox genes in embryogenesis and pathogenesis." *Pediatric research* 42.4 (1997)

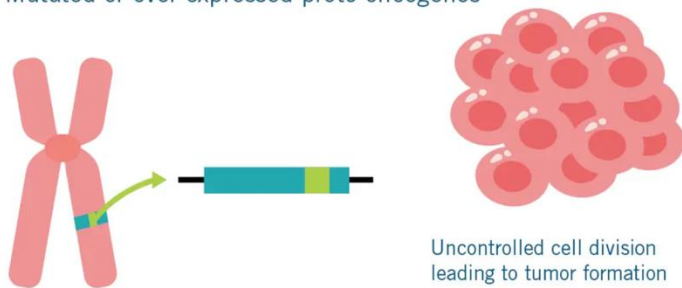
<https://www.rndsystems.com/cn/resources/articles/sonic-hedgehog-morphogen-involved-axon-guidance>

Direction of Causation: Cancer Research

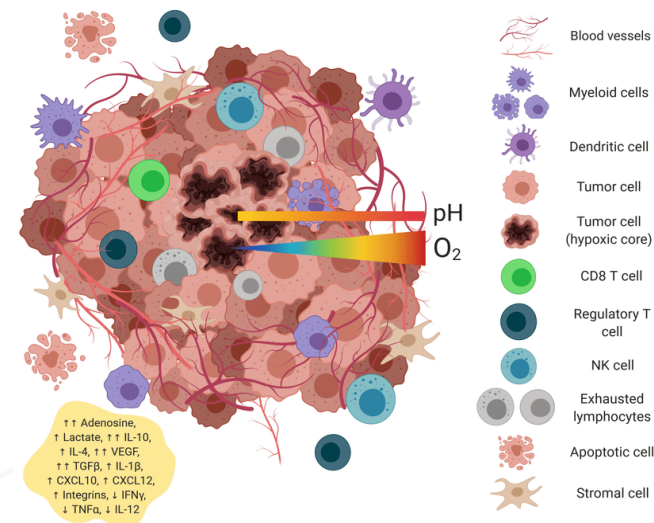
Reductionist, upward causation,
driver genes

Oncogene:

Mutated or over-expressed proto oncogenes



Holistic, downward causation,
tumour microenvironment

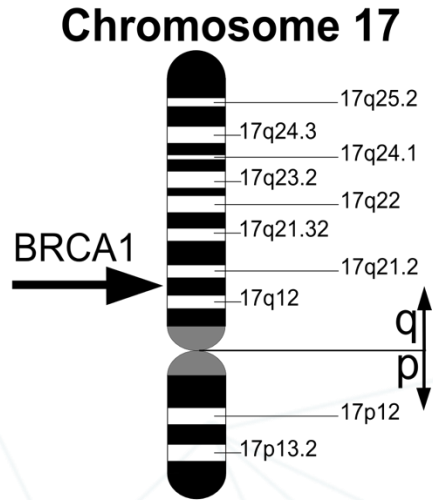


<https://biocare.net/blog/biocare-basics-oncogenes/>

Piñeiro Fernández, Julián, et al. "Hepatic tumor microenvironments and effects on NK cell phenotype and function"

The Controversies: BRCA Genes and Breast Cancer

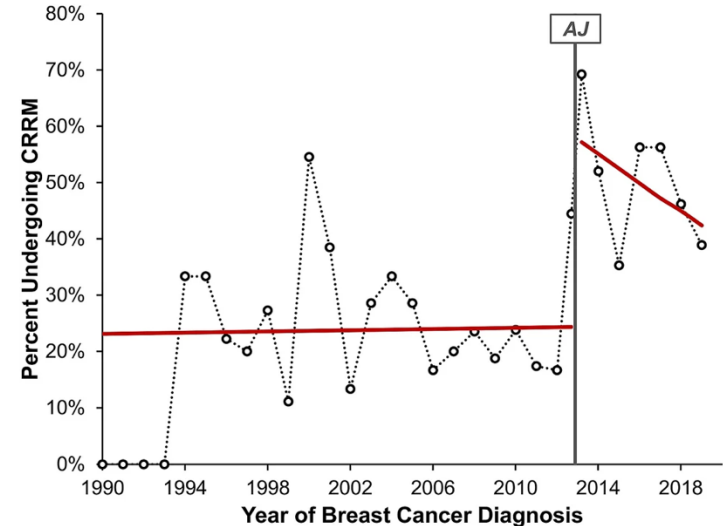
BRCA1 gene



Angelina Joley effect



Risk-reducing mastectomy trends in patients



Basu, Narendra Nath, et al. "The Angelina Jolie effect: contralateral risk-reducing mastectomy trends in patients at increased risk of breast cancer." *Scientific Reports* 11.1 (2021): 2847.

Conclusions: Complementary Approaches

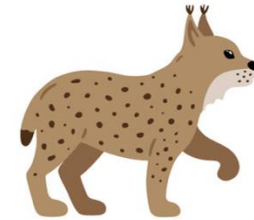
Reductionist Approach

- **Breaks** systems into parts for clear, reproducible cause-and-effect insights
- **Powers** most biological research, databases, and textbook knowledge
- **Limitations:** overlooks interactions, context-dependent behavior, and emergent properties

Holistic Approach

- **Examines** whole systems – interconnections, emergent phenomena, downward causation.
- **Essential** for understanding complex behaviors (e.g., cellular networks, ecosystems)
- **Limitations:** methods are still maturing; findings can be harder to interpret and apply. **Influenced** by reductionist tradition.

Thank you!



Questions



Maria Selifanova

Bioinformatician

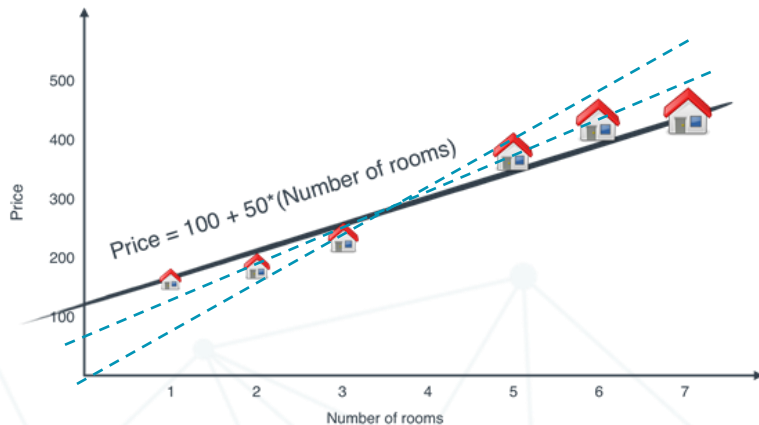
selifanovamariia@gmail.com

The background features a series of overlapping, curved shapes in various shades of blue and yellow. The shapes are semi-transparent, creating a layered effect. The colors transition from a deep blue on the left to a bright yellow on the right, with intermediate shades of teal and light blue in between.

Deep Learning: a Powerful Tool for Solving Mysteries of Life Sciences

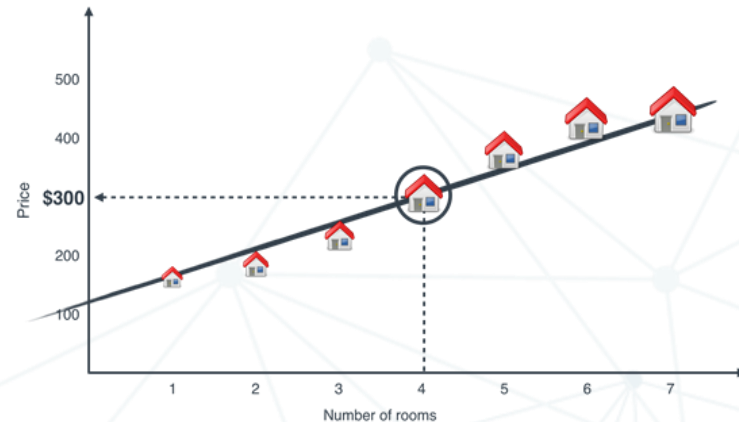
Machine learning (ML): Introduction

- Input: a **set of examples** (data) and a **task** to perform.
- Algorithm figures out how to accomplish the task based on the examples it's given (“**learning**” component).
- In ML, a machine **is not being explicitly programmed** to make predictions based on some set of pre-defined rules.



Training dataset:

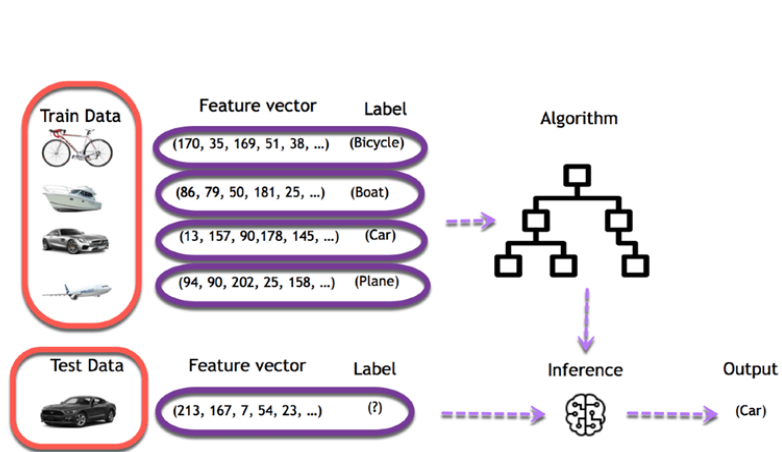
apartment price based on number of rooms



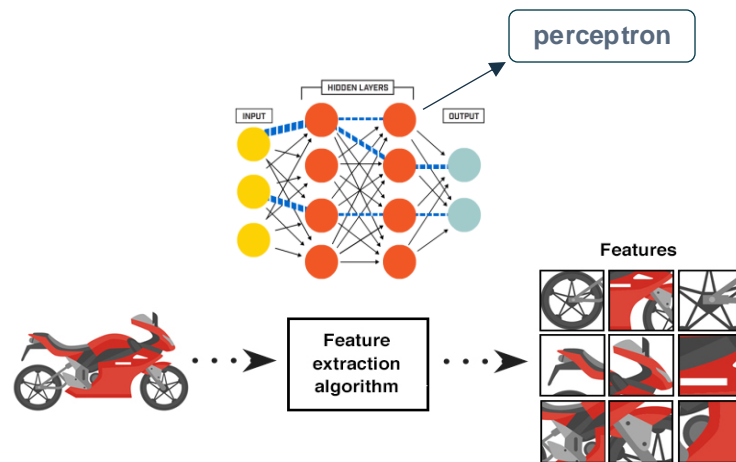
Prediction:

linear regression-based algorithm for an unknown sample

Machine Learning vs. Deep Learning

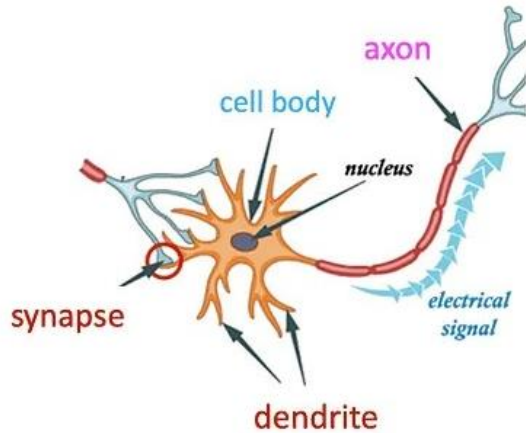


Machine Learning – statistical algorithms that can learn from data and generalize to unseen data; a feature vector is constructed **manually**

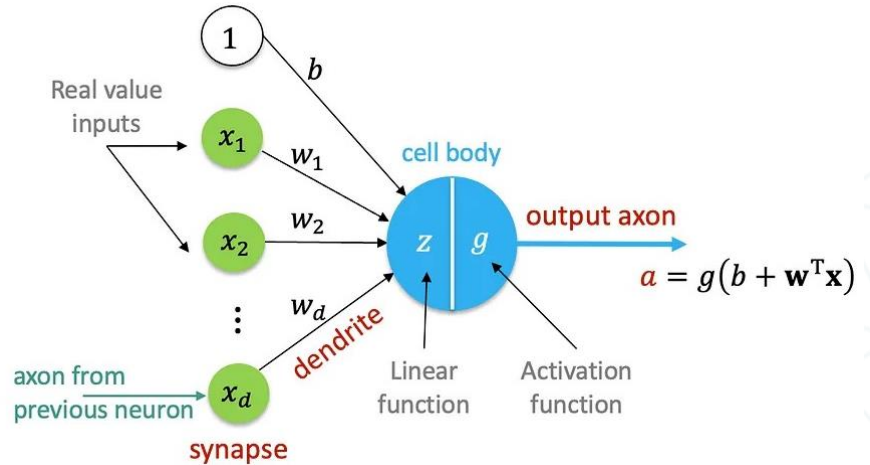


Deep Learning – a subset of machine learning using neural networks, which mimics the **network of neurons** inside a human brain; features are derived **automatically**

A Concept of Neural Network: Perceptron

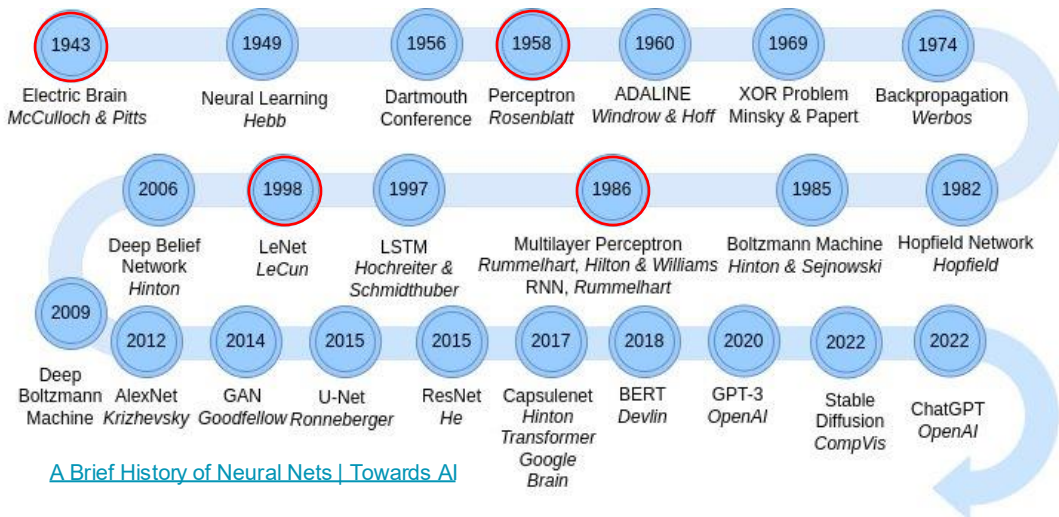


An **artificial neuron** can be thought of as a mathematical model that was influenced by a **biological neuron**



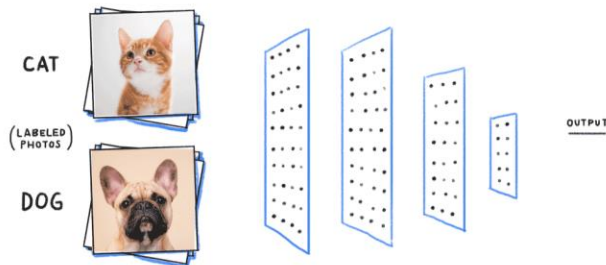
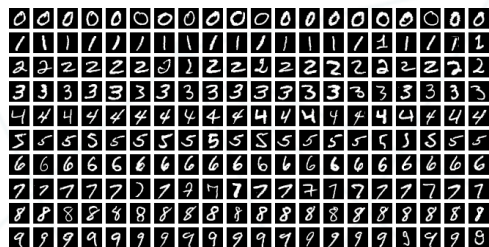
McCulloch-Pitts neuron, a groundbreaking concept introduced by Warren McCulloch and Walter Pitts in 1943 and developed by Frank Rosenblatt into a **Perceptron model in 1958**

Modern Neural Networks



[A Brief History of Neural Nets | Towards AI](#)

- DL applications:**
- Automatic translation
 - Text and speech recognition
 - Traffic prediction
 - Online fraud detection
 - Image recognition
 - Spam filtering



What is about Life Sciences?

Convolutional Neural Network (CNN): Blood Cells Classification (2024)

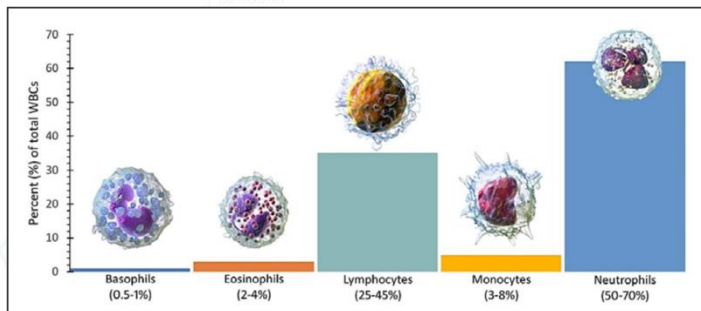
scientific reports

OPEN **White blood cells classification using multi-fold pre-processing and optimized CNN model**

Check for updates

Oumaima Saidani¹, Muhammad Umer², Nazik Alturki¹, Amal Alshardan¹, Muniba Kiran³, Shtwal Alsulbai¹, Tai-Hoon Kim^{4,5} & Imran Ashraf^{6,7}

White blood cells (WBCs) play a vital role in immune responses against infections and foreign agents. Different WBC types exist, and anomalies within them can indicate diseases like leukemia. Previous research suffers from limited accuracy and inflated performance due to the usage of less important features. Moreover, these studies often focus on fewer WBC types, exaggerating accuracy. This study addresses the crucial task of classifying WBC types using microscopic images. This study introduces a novel approach using extensive pre-processing with data augmentation techniques to produce a more significant feature set to achieve more promising results. The study conducts experiments employing both conventional deep learning and transfer learning models, comparing performance with state-of-the-art machine and deep learning models. Results reveal that a pre-processed feature set and convolutional neural network classifier achieves a significantly better accuracy of 0.99. The proposed method demonstrates superior accuracy and computational efficiency compared to existing state-of-the-art works.

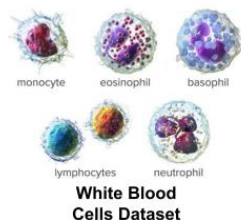
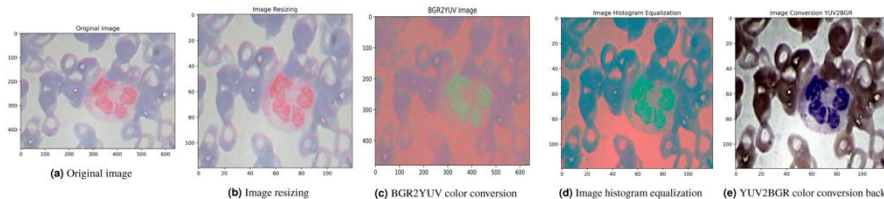


Saidani O. et al. White blood cell classification using multi-fold pre-processing and optimized CNN model. *Scientific Reports*, 14, 3570 (2024)

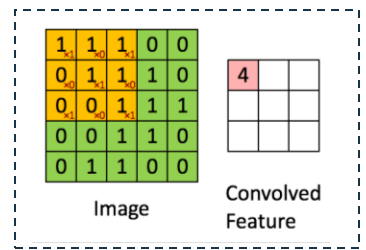
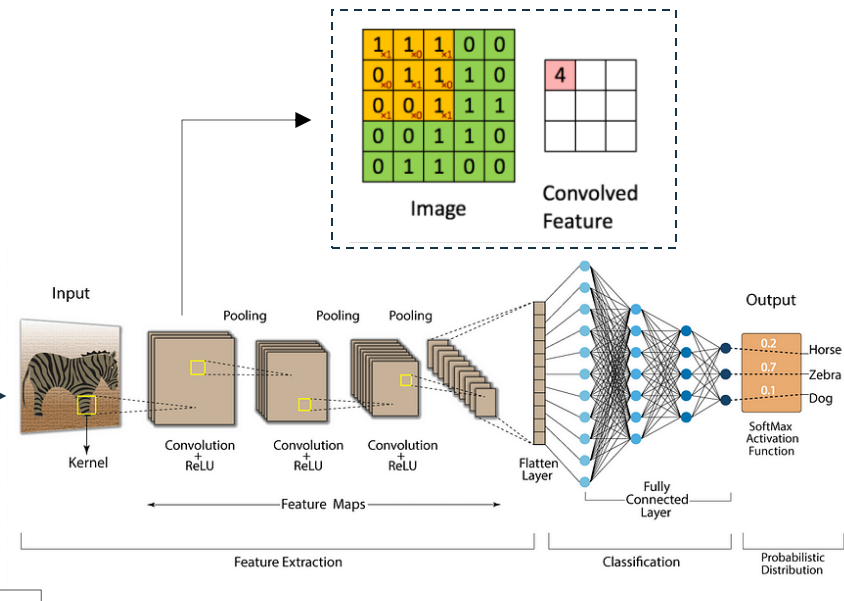
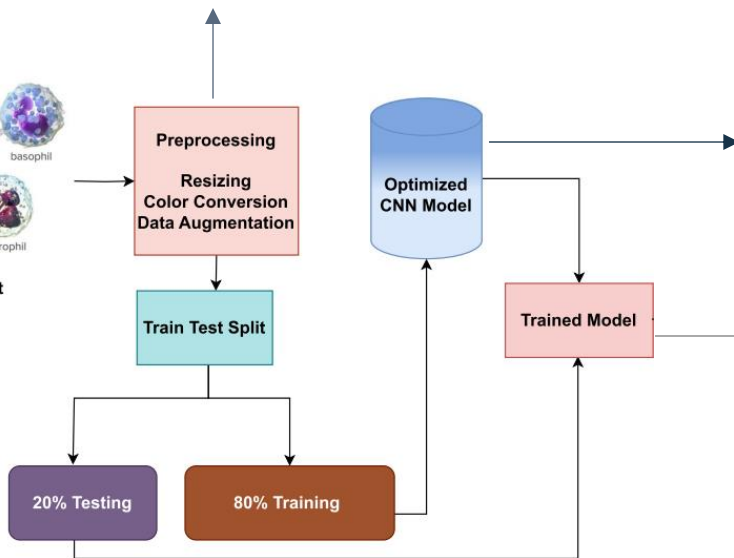
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This study addresses the crucial task of classifying WBC types using microscopic images. This study introduces a novel approach using extensive pre-processing with **data augmentation** techniques to produce a more significant feature set to achieve more promising results. The study conducts experiments employing both conventional deep learning and transfer learning models, comparing performance with state-of-the-art machine and deep learning models. Results reveal that a pre-processed feature set and convolutional neural network classifier achieves a significantly better accuracy of 0.99.

Convolutional Neural Network (CNN): Proposed Solution



White Blood Cells Dataset



Evaluation
 Accuracy
 Precision
 Recall
 F-score

Classifier	Accuracy	Precision	Recall	F1 score
VGG16	0.9609	0.96	0.96	0.96
InceptionV3	0.9720	0.97	0.97	0.97
MobileNetV2	0.7847	0.78	0.78	0.78
ResNET50	0.7458	0.81	0.74	0.73
Proposed CNN	0.9986	0.99	0.99	0.99

Generative Pretrained Transformer (GPT): ChemCrow (2024)



nature machine intelligence



Article

<https://doi.org/10.1038/s42256-024-00832-8>

Augmenting large language models with chemistry tools

Received: 13 September 2023

Accepted: 27 March 2024

Published online: 08 May 2024

Check for updates

Andres M. Bran^{1,2,6}, Sam Cox^{3,4,6}, Oliver Schilter^{1,2,5}, Carlo Baldassari⁵, Andrew D. White^{3,4} & Philippe Schwaller^{1,2} ✉

Large language models (LLMs) have shown strong performance in tasks across domains but struggle with chemistry-related problems. These models also lack access to external knowledge sources, limiting their usefulness in scientific applications. We introduce ChemCrow, an LLM chemistry agent designed to accomplish tasks across organic

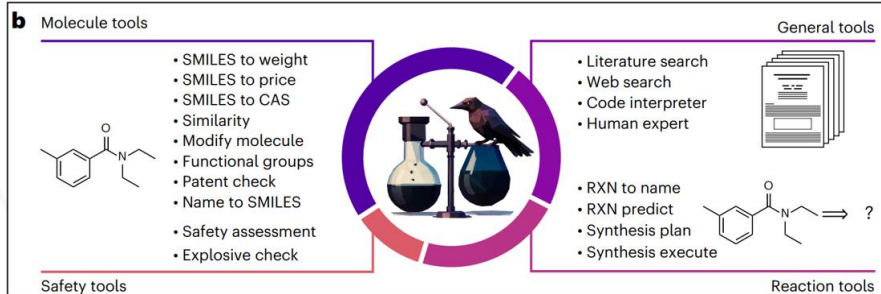
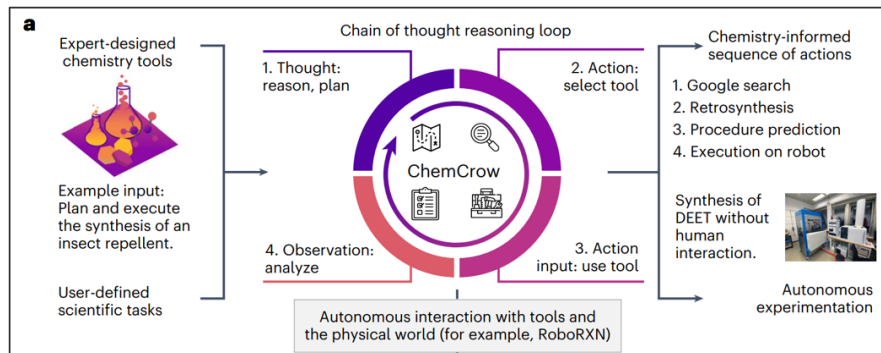
The screenshot shows the ChemCrow interface. On the left, there's a sidebar with the ChemCrow logo and a list of 12 available tools, including PatentCheck, MolSimilarity, SMILES2Weight, and FunctionalGroups. The main chat window shows a user input: "The reaction of phytic acid with acetyl chloride does not seem to produce any new product, as the output SMILES is the same as the input for phytic acid. Now, I will predict the product of genistein with acetyl chloride." The system response includes the action "R2N.Predict" and the SMILES string "CC(=O)OCl.ccc(-c2cc3cc(OC(C)=O)cc(O)c3c2=O)cc1". Below the text, a chemical reaction diagram shows the reaction of phytic acid with acetyl chloride to form a product.

Bran A. M. et al. Augmenting large language models with chemistry tools. *Nature Machine Intelligence* (2024)

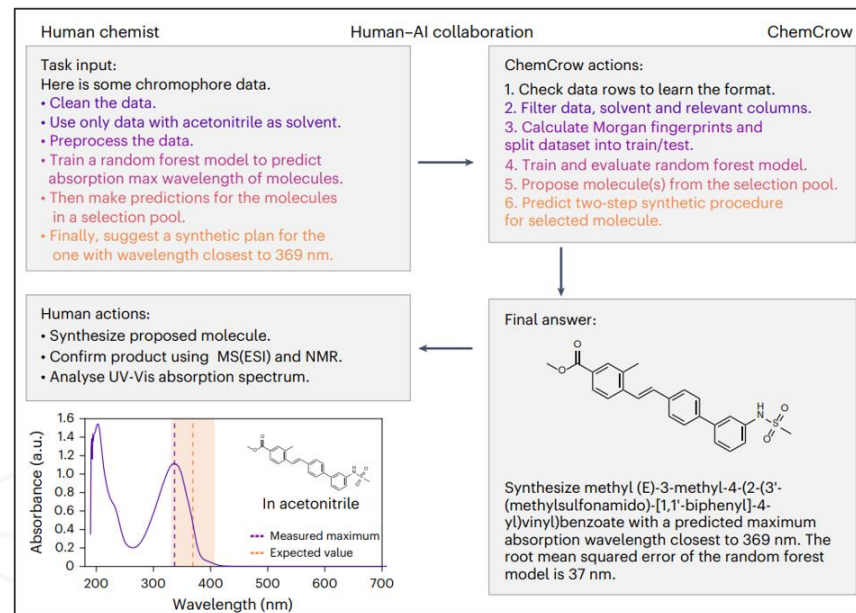
Large language models (LLMs) have shown strong performance in tasks across domains but struggle with chemistry-related problems. These models also **lack access to external knowledge sources**, limiting their usefulness in scientific applications.

We introduce ChemCrow, an LLM chemistry agent designed to **accomplish tasks across organic synthesis, drug discovery and materials design**. By integrating 18 expert-designed tools and using GPT-4 as the LLM, ChemCrow augments the LLM performance in chemistry, and new capabilities emerge. Our agent autonomously planned and executed the syntheses of an insect repellent and three organocatalysts and guided the discovery of a novel chromophore. Our evaluation, including both LLM and expert assessments, demonstrates ChemCrow's effectiveness in **automating a diverse set of chemical tasks**.

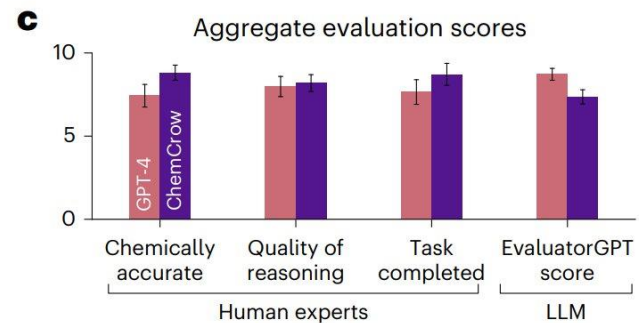
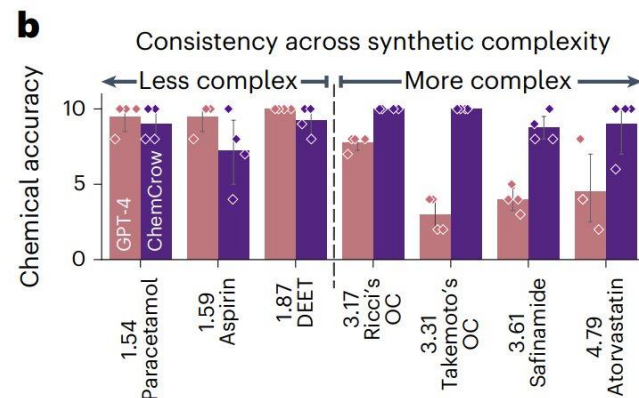
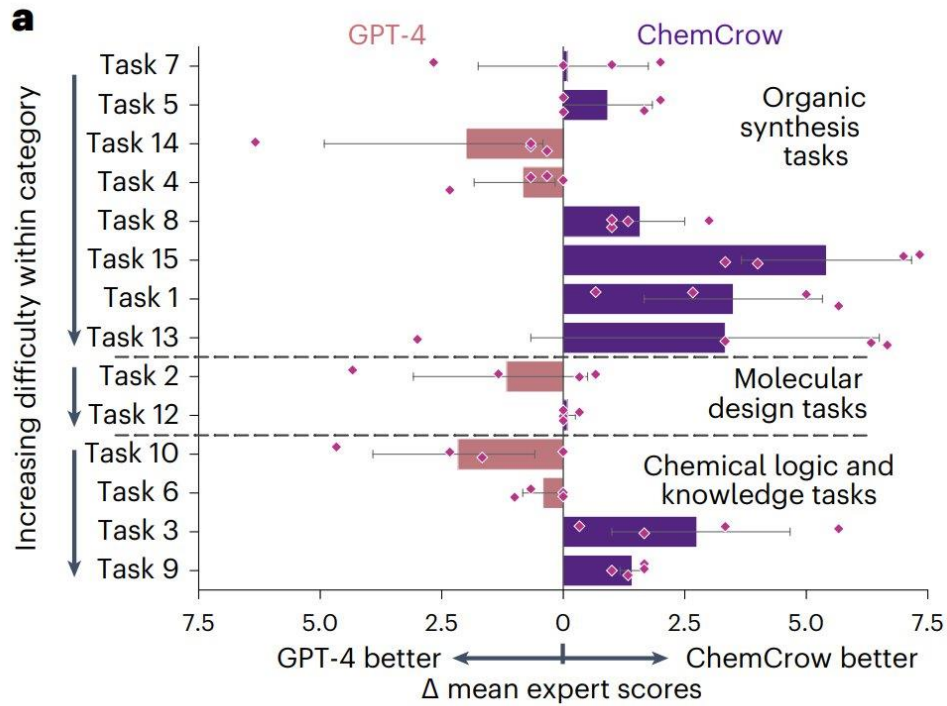
Generative Pretrained Transformer (GPT): Workflow



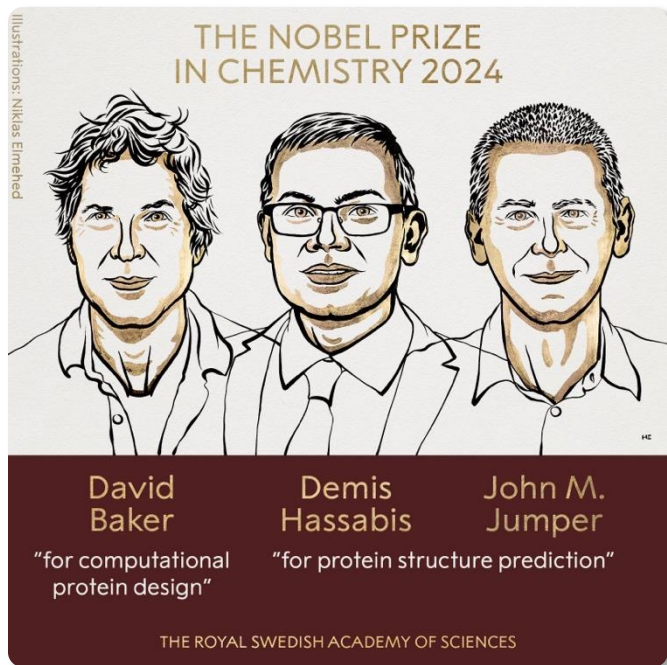
Human-model interaction leading to the discovery of a new chromophore:



Generative Pretrained Transformer (GPT): Results



AlphaFold 2020-2024

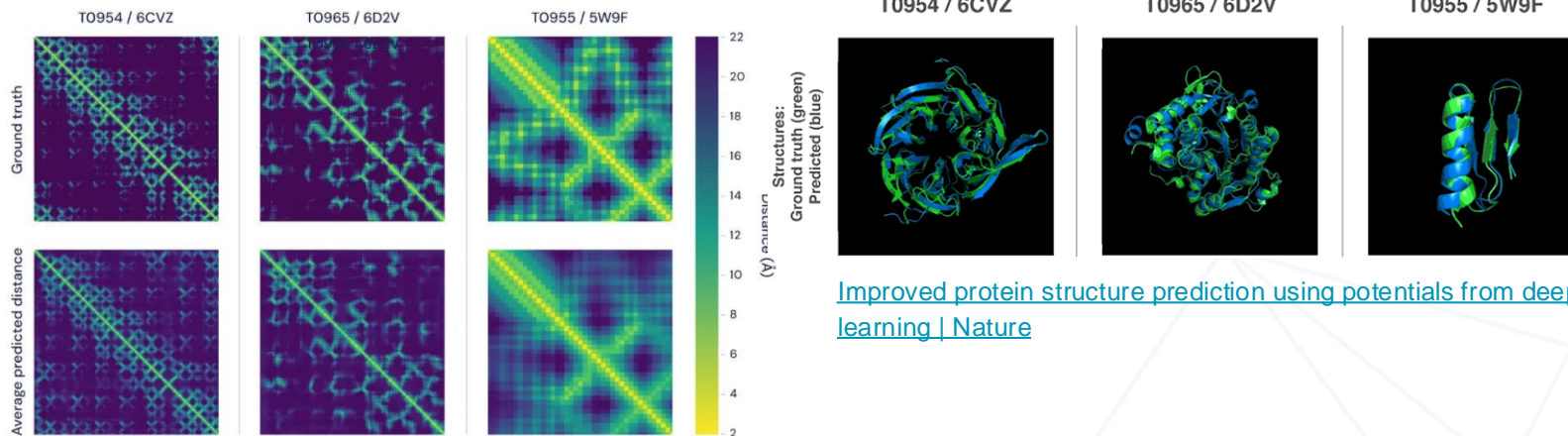


AlphaFold (2020) – CNN-based solution for prediction of the distances between pairs of residues. The resulting potential is optimized by a simple gradient descent algorithm to generate structures without complex sampling procedures. Won CASP13 competition.

AlphaFold2 (2021) – first computational method that can regularly predict protein structures with atomic accuracy even in cases in which no similar structure is known. Won CASP14 competition.

AlphaFold3 (2024) – diffusion-based architecture, which is capable of joint structure prediction of complexes including proteins, nucleic acids, small molecules, ions, and modified residues. Nobel prize in Chemistry.

AlphaFold2 (2020): Results



[Improved protein structure prediction using potentials from deep learning | Nature](#)

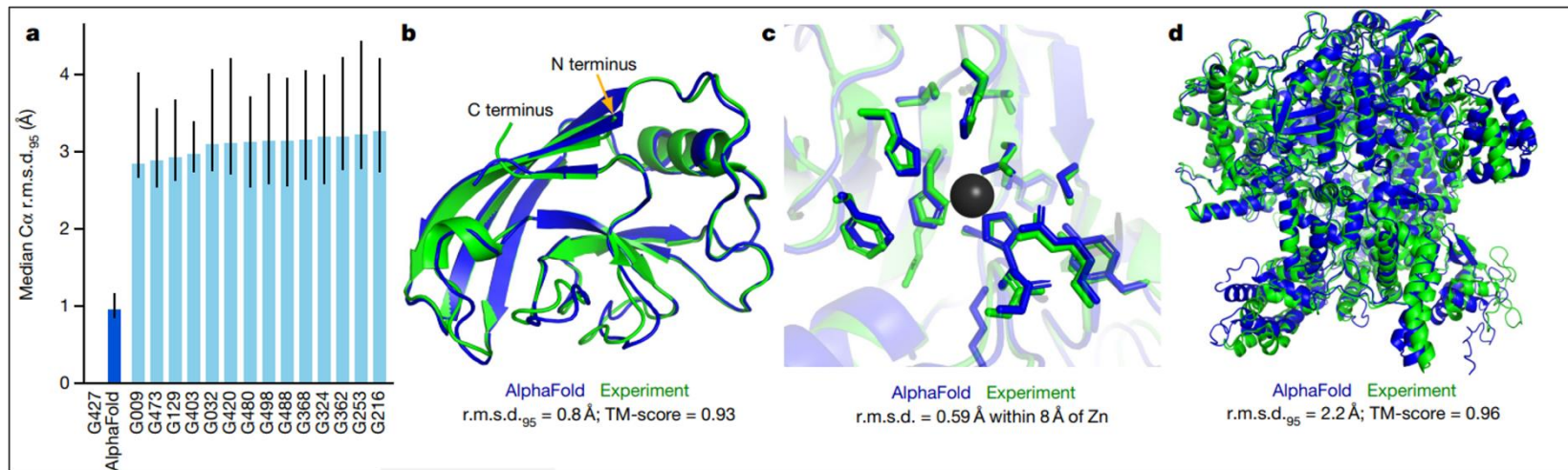
Two ways of visualizing the accuracy of AlphaFold's predictions

The left figure features the distance matrices for three proteins. The brightness of each pixel represents the distance between the amino acids in the sequence comprising the protein—the brighter the pixel, the closer the pair. Shown in the top row are the real, experimentally determined distances, and in the bottom row, the average of AlphaFold's predicted distance distributions. Importantly, these match well on both global and local scales.

The right panels represent the same comparison using 3D models, featuring AlphaFold's predictions (blue) versus ground-truth data (green) for the same three proteins.

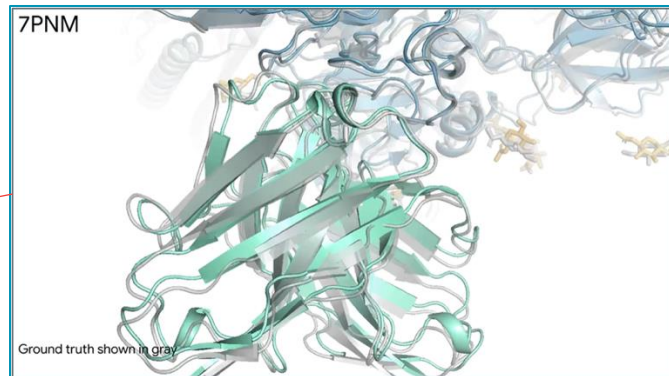
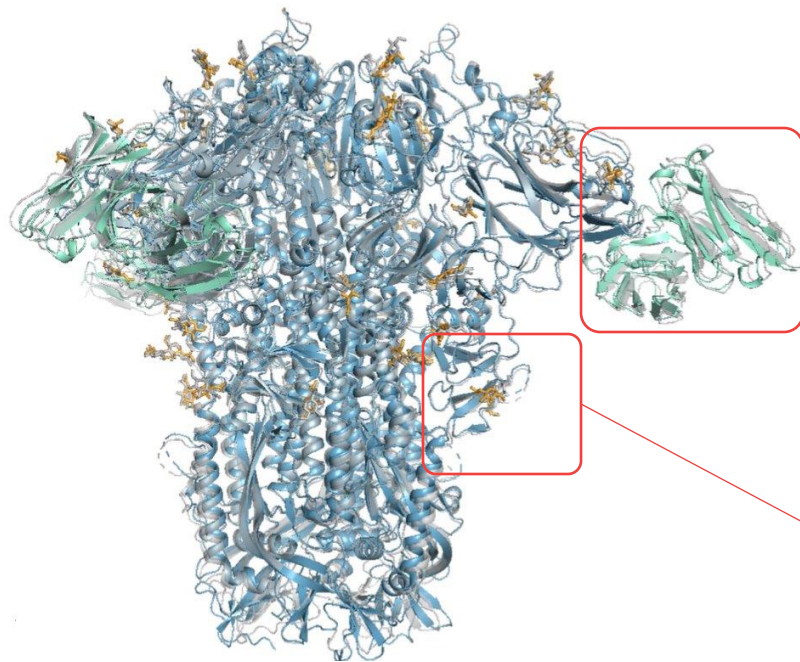
AlphaFold2 (2021): Results

[Highly accurate protein structure prediction with AlphaFold | Nature](#)

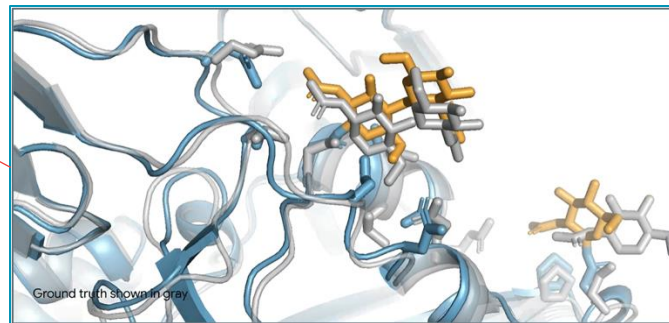


- a) The performance of AlphaFold on the CASP14 dataset (n = 87 protein domains) relative to the top-15 entries (out of 146 entries);
- b) AlphaFold2 prediction of CASP14 target T1049 (PDB 6Y4F, blue) compared with the experimental structure (green).
- c) CASP14 target T1056 (PDB 6YJ1). An example of a well-predicted zinc-binding site (AlphaFold has accurate side chains even though it does not explicitly predict the zinc ion);
- d) CASP target T1044 (PDB 6VR4) - a 2,180-residue single chain - was predicted with correct domain packing.

AlphaFold3 (2024): Results



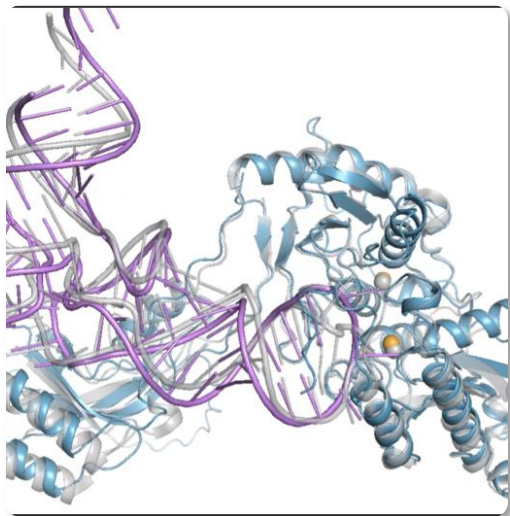
[Accurate structure prediction of biomolecular interactions with AlphaFold 3 | Nature](#)



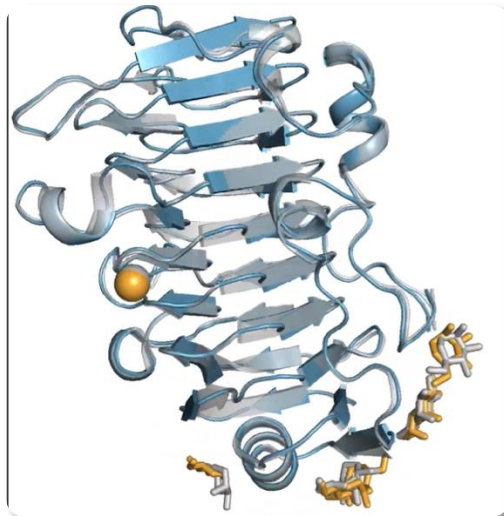
7PNM - Spike protein of a common cold virus (Coronavirus OC43)

AlphaFold 3's structural prediction for a spike protein (blue) of a cold virus as it interacts with antibodies (turquoise) and simple sugars (yellow), accurately matches the true structure (gray).

AlphaFold3 (2024): Results



8AW3 - RNA modifying protein: AlphaFold 3's prediction for a molecular complex featuring a protein (blue), a strand of RNA (purple), and two ions (yellow) closely matches the true structure (gray). This complex is involved with the creation of other proteins — a cellular process fundamental to life and health.



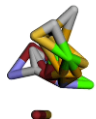
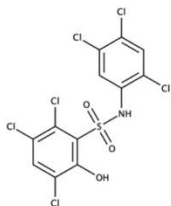
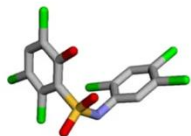
7BBV - Enzyme: AlphaFold 3's prediction for a molecular complex featuring an enzyme protein (blue), an ion (yellow sphere) and simple sugars (yellow), along with the true structure (gray). This enzyme is found in a soil-borne fungus (*Verticillium dahliae*) that damages a wide range of plants.



7R6R - DNA binding protein: AlphaFold 3's prediction for a molecular complex featuring a protein (blue) bound to a double helix of DNA (pink) is a near-perfect match to the true molecular structure discovered through painstaking experiments (gray).

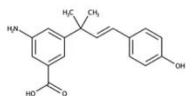
From SMILES to Graphs: ML-Driven Cheminformatics

Reference Structure

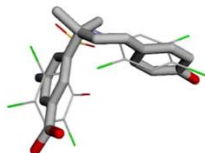


Generated Samples

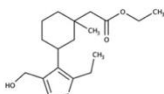
Sample 1



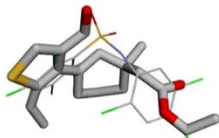
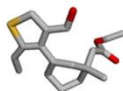
Tanimoto score
0.62



Sample 2

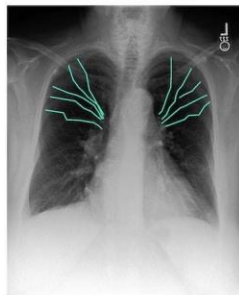


Tanimoto score
0.54

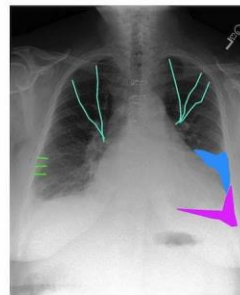


Explainable AI for Medical Image Analysis: Pulmonary Edema Case Study

(a) Vascular congestion



(b) Interstitial edema



(c) Alveolar edema



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Questions



Karina Pats

ML Engineer

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- **Senior Machine Learning Engineer**



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