AI and Structural Biology

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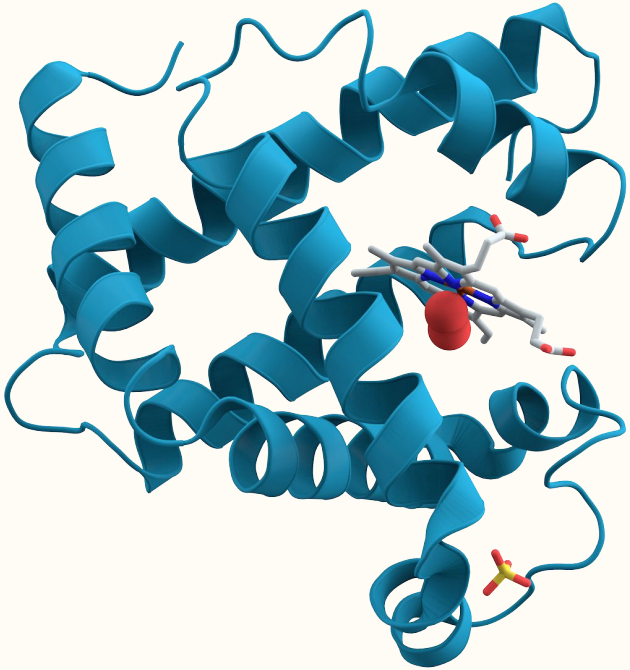
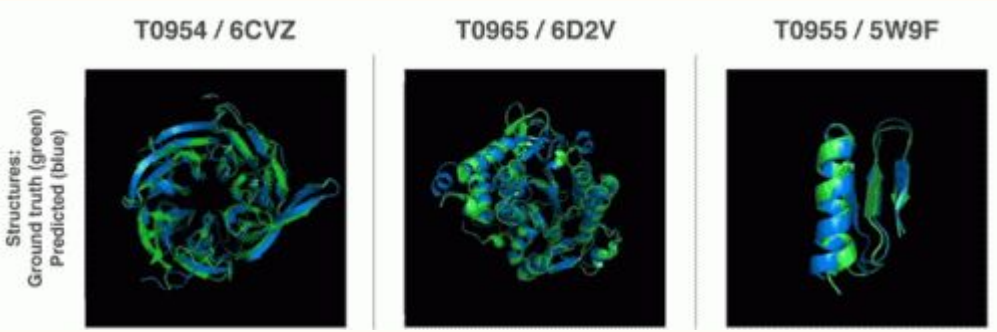
Table of Contents



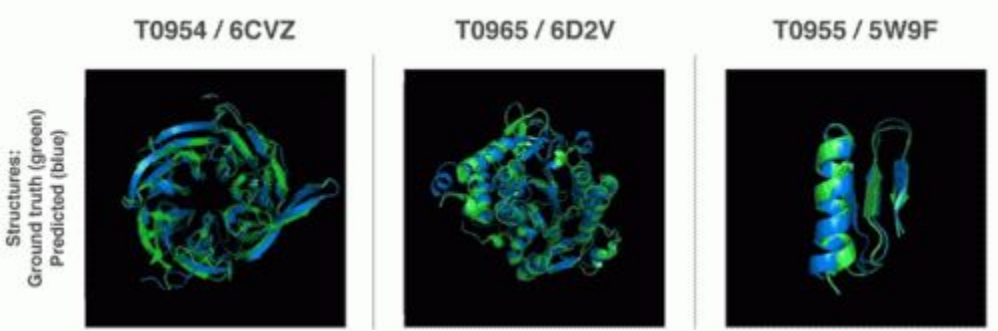
Structural Biology

The study of the three-dimensional structures of biological molecules, like proteins and nucleic acids, and how these structures relate to their functions. It aims to understand how molecules are built and how their shapes determine their biological activities.



Structural Biology

Our presentation will specifically focus on the critical role of structural biology in understanding **protein folding**, the process by which proteins acquire their intricate three-dimensional structures.



Protein Folding

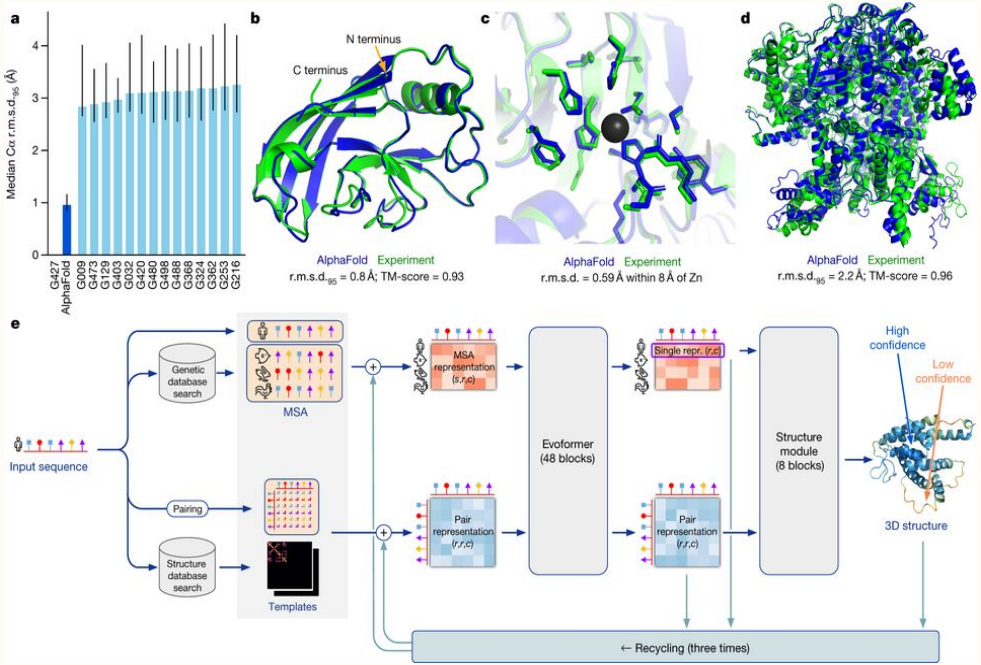
Protein folding is the physical process by which a protein chain acquires its native three-dimensional structure, a conformation that is typically biologically functional, from a random coil.

Importance

Protein folding is crucial because a protein's function is directly dependent on its specific 3D structure. Mis-folded proteins are implicated in various diseases (e.g., Alzheimer's, Parkinson's, cystic fibrosis), making accurate structure prediction vital for drug discovery and understanding biological processes. Historically, determining protein structures was a time-consuming and expensive experimental challenge.

AlphaFold

DeepMind Introduces AlphaFold: In 2018 and significantly advanced in 2020, DeepMind introduced AlphaFold, an AI system that predicts protein structures with unprecedented accuracy



State of Protein Folding Before AlphaFold

Before AlphaFold, accurate protein structure prediction was a "grand challenge" in biology. Experimental methods (like X-ray crystallography, NMR, cryo-EM) were the primary means, but they were often slow and not universally applicable. Computational methods existed but struggled to achieve experimental-level accuracy.

State of Protein Folding After AlphaFold

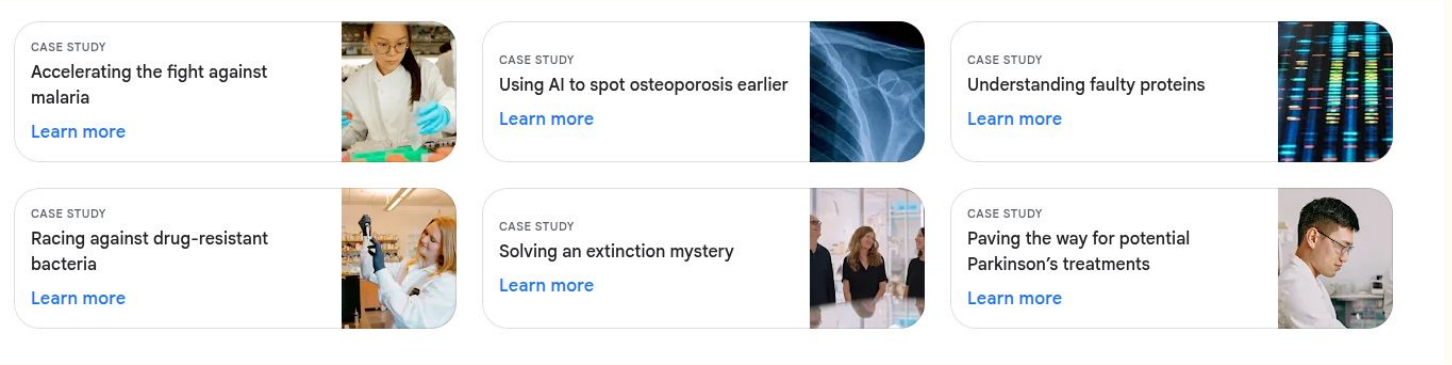
AlphaFold revolutionized the field. It can predict protein structures with near-experimental accuracy in a fraction of the time, making structural data accessible for a vast number of proteins that were previously intractable. This has accelerated research across numerous biological disciplines.

> “It normally takes four years to identify and characterise one of these small proteins. With the help of AlphaFold we managed 23 in a few months.

PROFESSOR RENIER VAN DER HOORN
UNIVERSITY OF OXFORD

How Researchers are using AlphaFold

Researchers are using AlphaFold to understand disease mechanisms, design new drugs, engineer novel enzymes, study protein-protein interactions, and even explore the structures of proteins from obscure organisms.



Beyond AlphaFold

1. **SKYCovione:** SKYCovione was the **world's first fully approved medicine created using computational protein design.** The COVID-19 vaccine that was famously **computationally designed** by researchers at the **University of Washington's Institute for Protein Design**, led by **David Baker.**

COVID-19 shots with Seattle origins reach regulatory milestones in South Korea, India

Beyond AlphaFold

1. **De Novo Drug Design:** Generative AI models (like GANs, VAEs, and diffusion models) can design novel molecules with desired properties (e.g., binding affinity, solubility, bioavailability) from scratch

De novo design of protein structure and function with RFdiffusion

What future looks like?

Within 5 years:

- **De Novo Protein and Enzyme Design:** Beyond natural proteins, AI will enable the routine design of custom proteins and enzymes for industrial applications (e.g., sustainable biofuels, biodegradable plastics, enhanced agricultural yields) and therapeutic uses. This will move from niche research to widespread application.
- **Advanced Vaccine and Diagnostic Development:** The success of computationally designed vaccines (like SKYCovione) will spur further development of highly effective and rapidly deployable vaccines and diagnostics for emerging pathogens.

- **Personalized Medicine:** AI will analyze individual patient genomic, proteomic, and clinical data to predict drug response and tailor treatment plans, leading to more effective therapies with fewer side effects.

- **Repurposing Existing Drugs:** AI will be increasingly used to identify new uses for existing, approved drugs, a faster and less expensive route to new treatments.

Thank you

Questions?