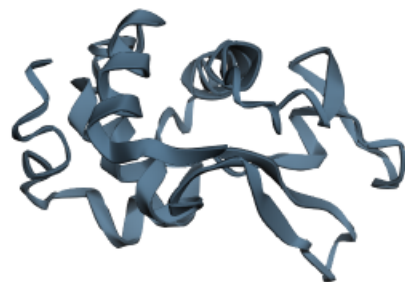


L7

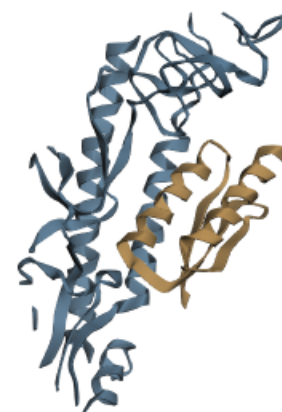
AI for Discovery and Invention

Case Study: Protein Prediction and Design

(K) (V) (F) (E) (R) ... →



Prediction



Design

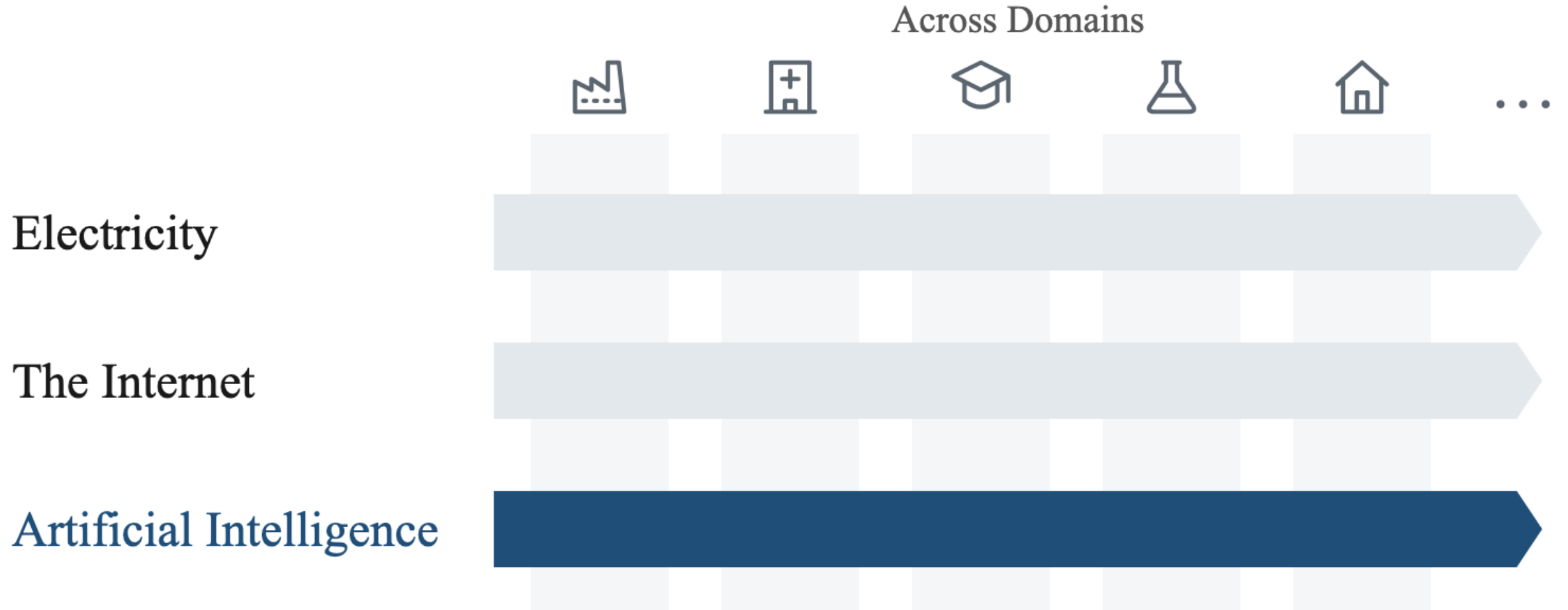
AILT1001

Artificial Intelligence Literacy I



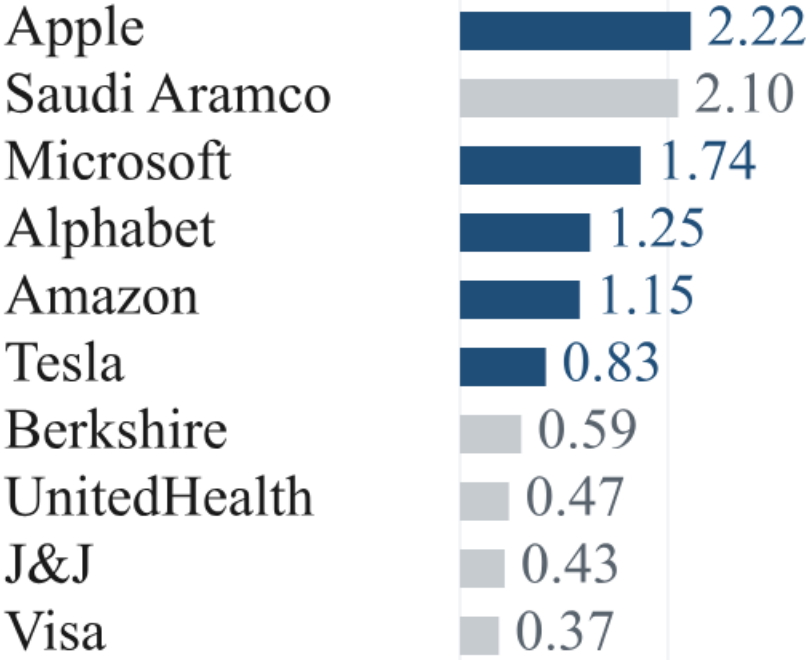
DEMO 1 · L6 Exit Ticket Results

AI as a Horizontal Enabling Layer

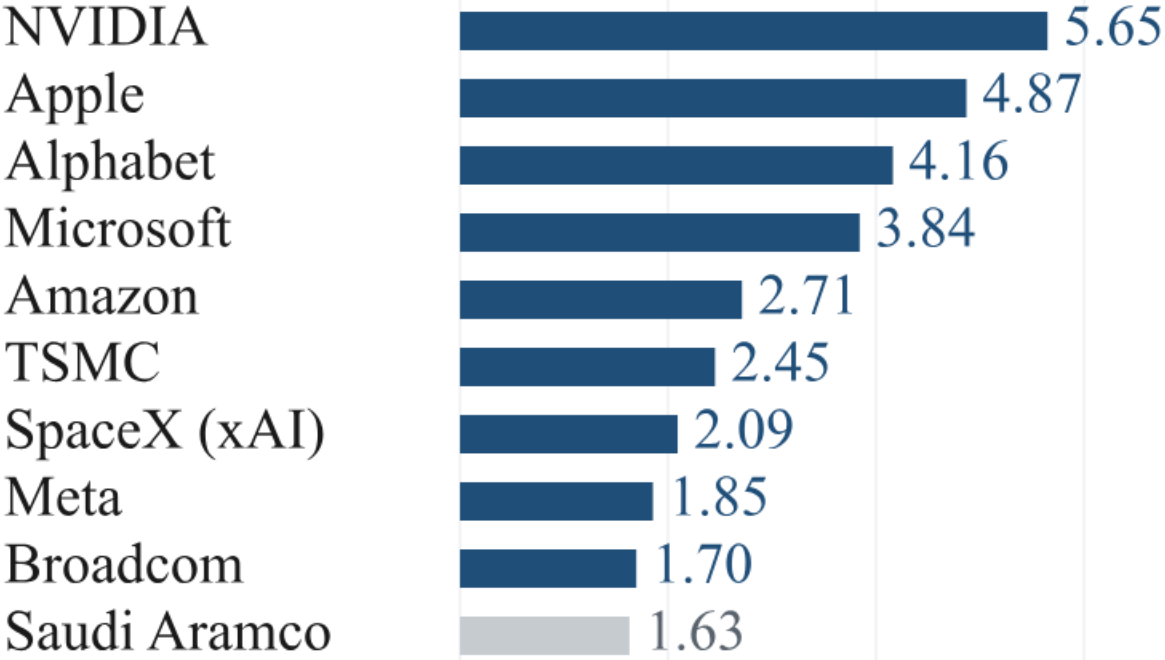


Top Ten Companies by Market Cap

October 2022



October 2026



Market Cap: \$11.2T → \$31.0T (2.78×)

US\$ Trillion





Proteins Make Life Work

Examples of Protein Functions

Movement



Muscle proteins help you move

Digestion

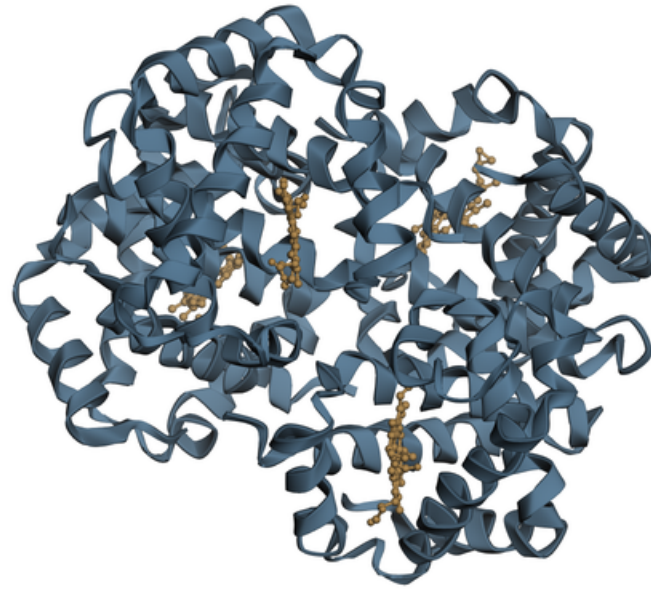


Enzymes break down food

Defence



Antibodies recognise threats



Transport



Hemoglobin carries oxygen

Signalling



Insulin regulates blood glucose

Support



Collagen supports tissues

A protein's shape helps it do its job

Protein Folding

Amino Acids



Select a Letter



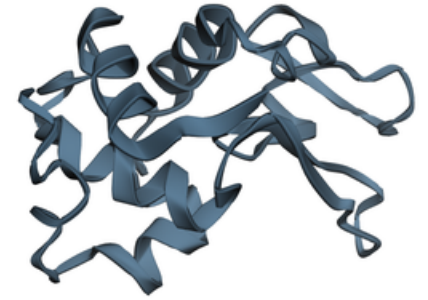
Sequence

K	V	F	E	R	C	E	L	A	R	T	L	K
R	L	G	M	D	G	Y	R	G	I	S	L	A
N	W	M	C	L	A	K	W	E	S	G	Y	N
T	R	A	T	N	Y	N	A	G	D	R	S	T
D	Y	G	I	F	Q	I	N	S	R	Y	W	C
N	D	G	K	T	P	G	A	V	N	A	C	H
L	S	C	S	A	L	L	Q	D	N	I	A	D
A	V	A	C	A	K	R	V	V	R	D	P	Q
G	I	R	A	W	V	A	W	R	N	R	C	Q
N	R	D	V	R	Q	Y	V	Q	G	C	G	V

Human Lysozyme



Protein Shape

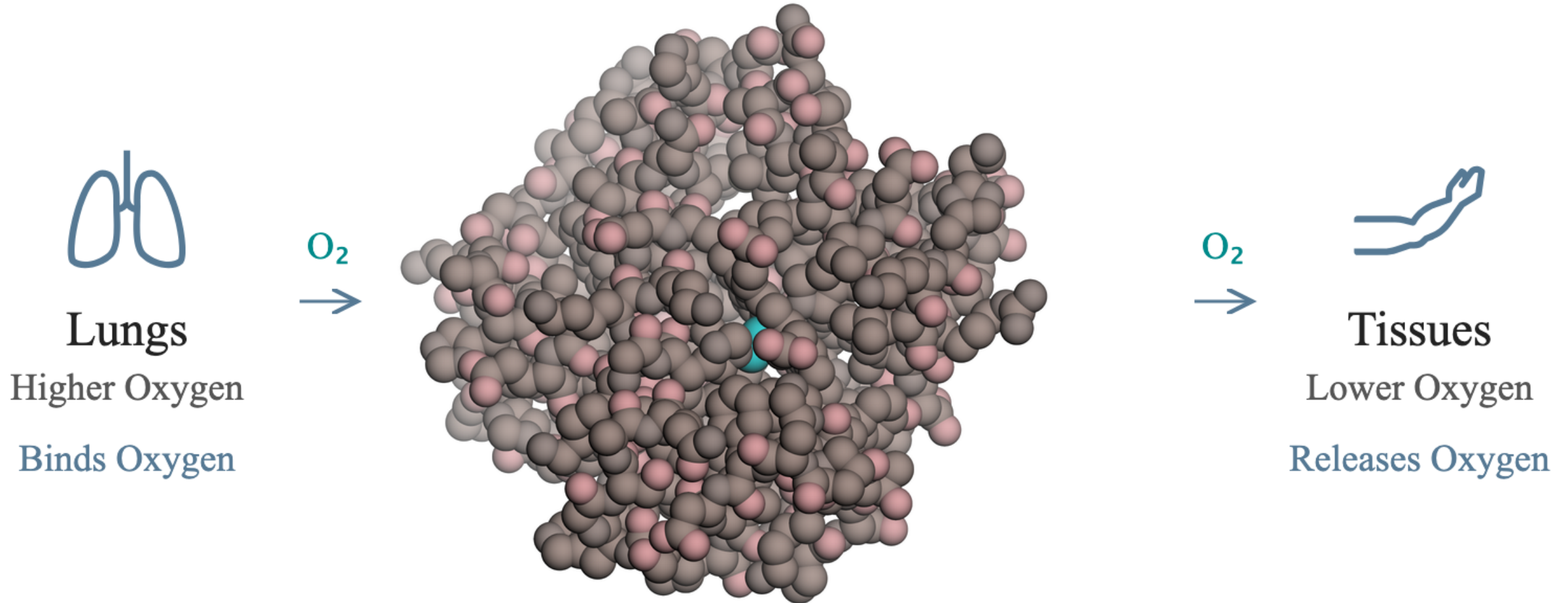


Ribbon = Backbone

Given the sequence, can we predict the shape?

Shape Enables Function

Hemoglobin carries oxygen from lungs to tissues



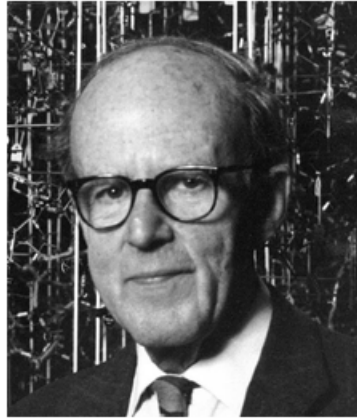
Finding a Structure Took Years

From experimental measurements to a 3D model

X-Ray Crystallography



John Kendrew
Myoglobin
1958



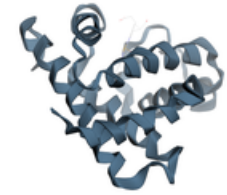
Max Perutz
Hemoglobin
1960



Crystal



Diffraction



Structure

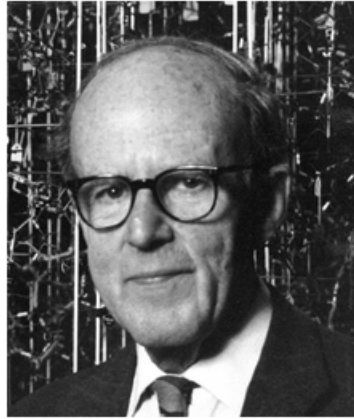
Finding a Structure Took Years

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John Kendrew
Myoglobin
1958



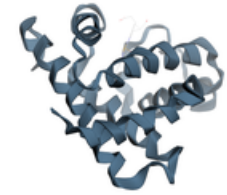
Max Perutz
Hemoglobin
1960



Crystal



Diffraction



Structure

12 Years

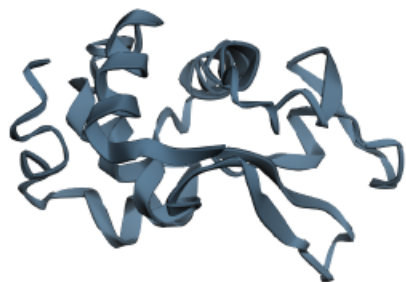
For Myoglobin's First Structure

~100 Entries

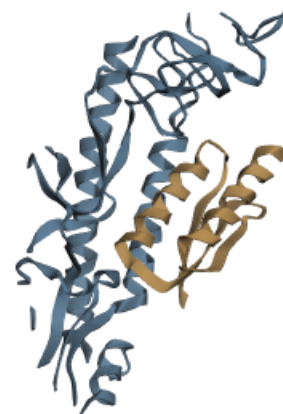
In the PDB by 1982

Case Study: Protein Prediction and Design

(K) (V) (F) (E) (R) ... →



Prediction



Design

Predicting and Testing Protein Structures

How do we know a predicted structure is right?

Sequence

Prediction

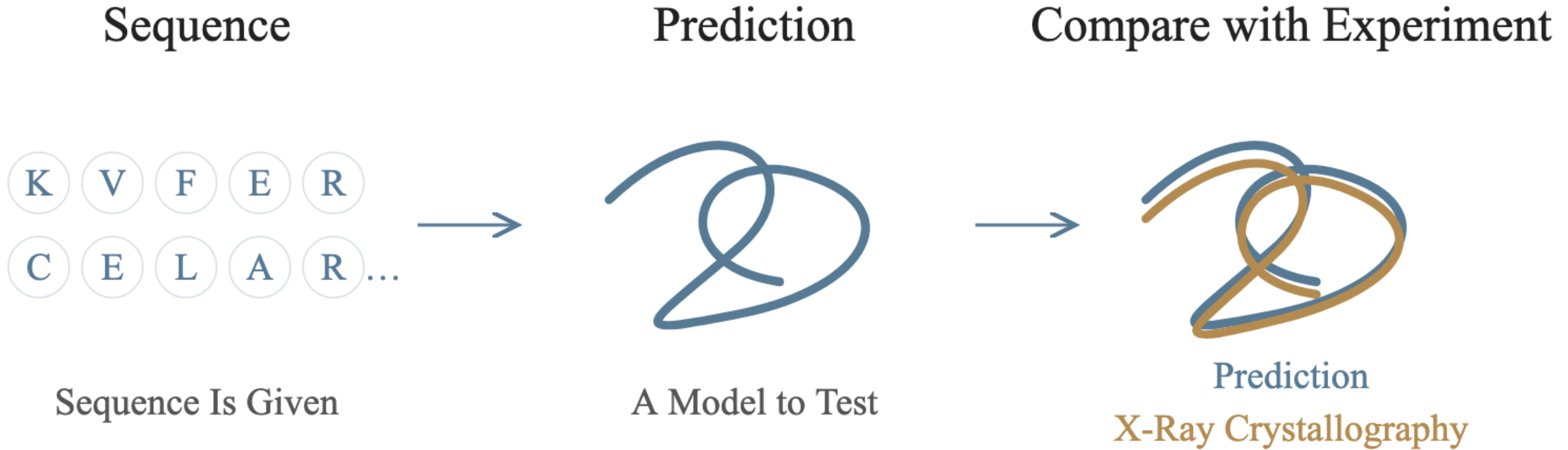


Sequence Is Given

A Model to Test

Predicting and Testing Protein Structures

How do we know a predicted structure is right?



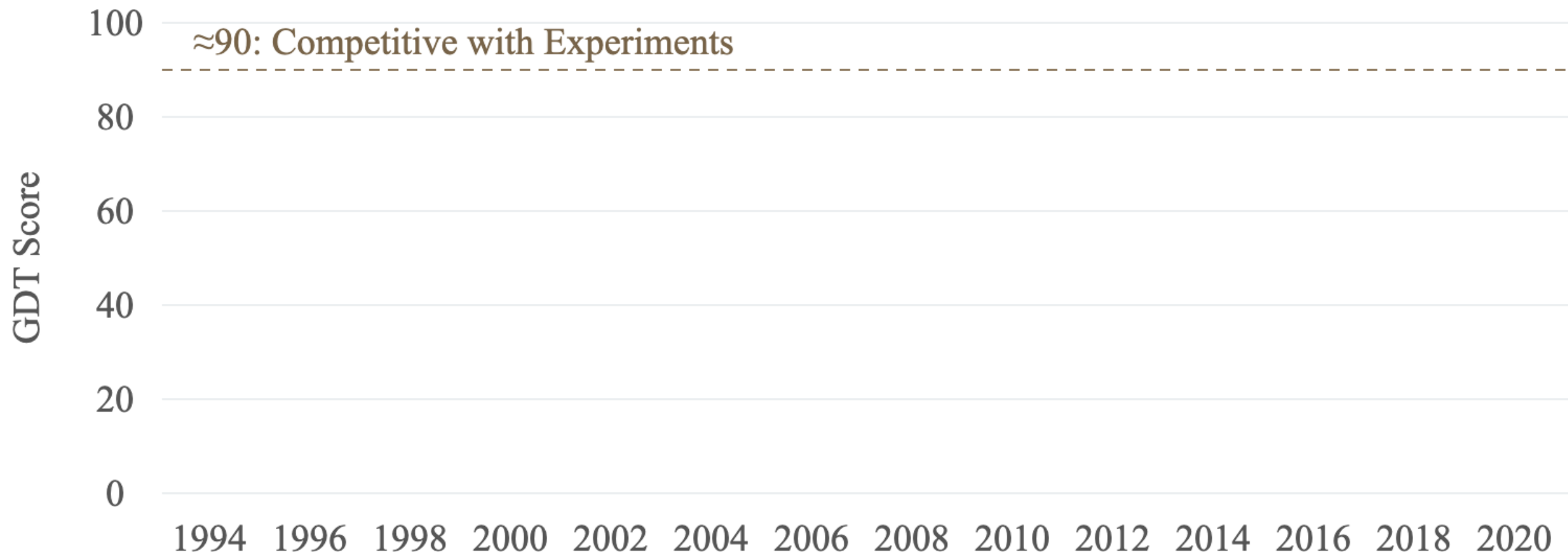
CASP: A Structure Prediction Competition

Predict Before Seeing the Experimental Structure

Global Distance Test (GDT): Higher Score = Closer Match

CASP: Decades of Progress

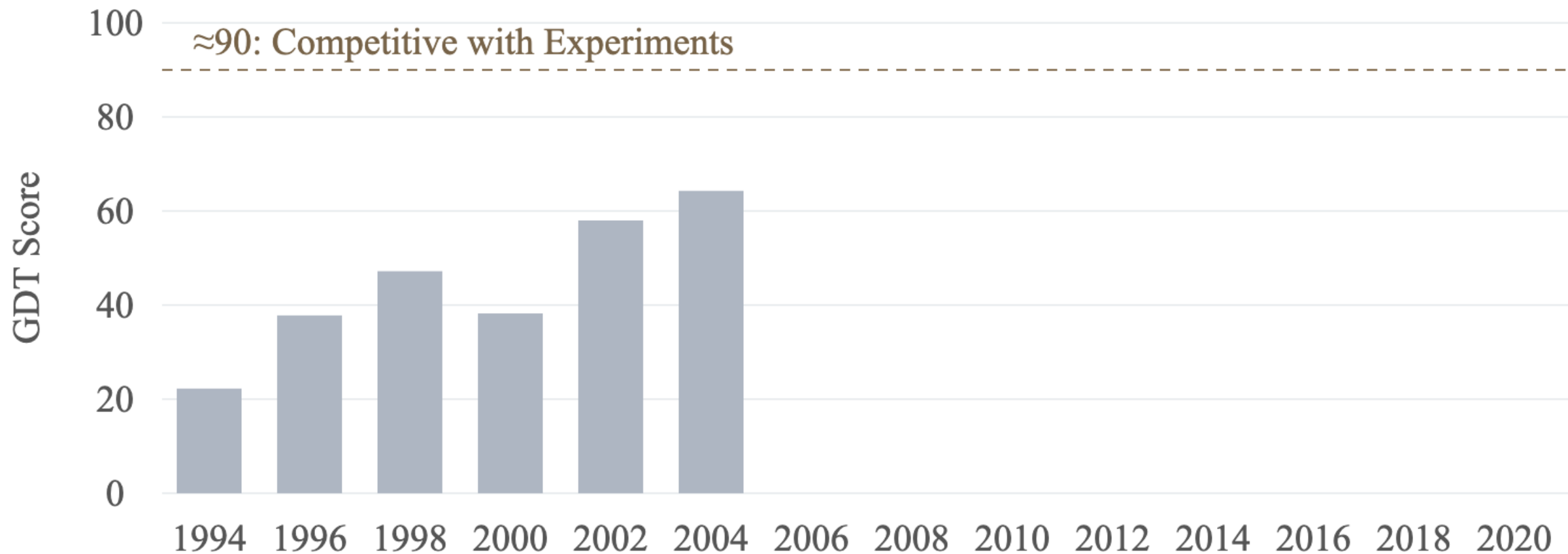
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

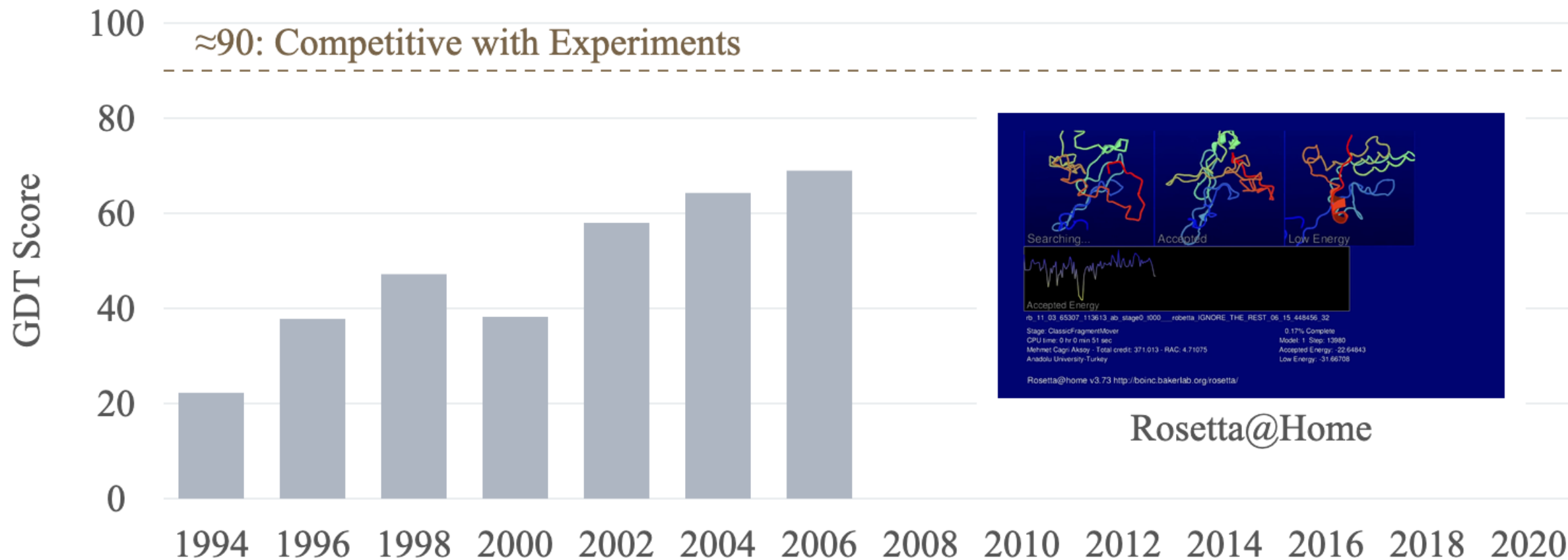
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

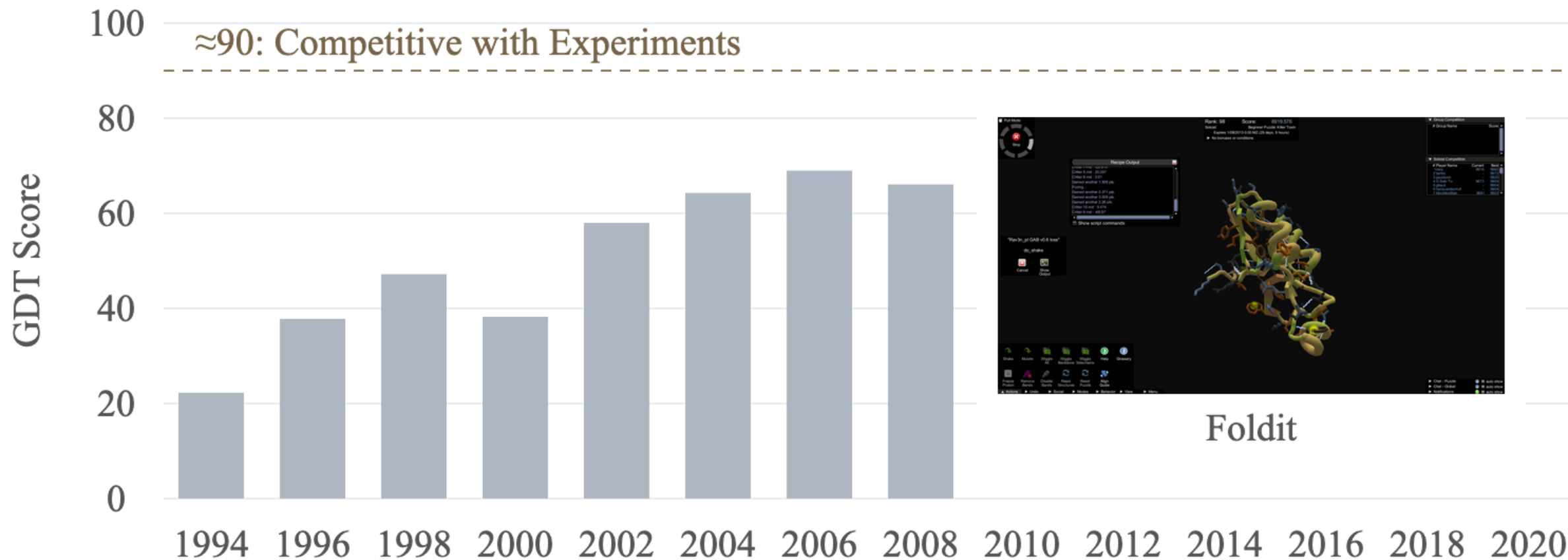
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

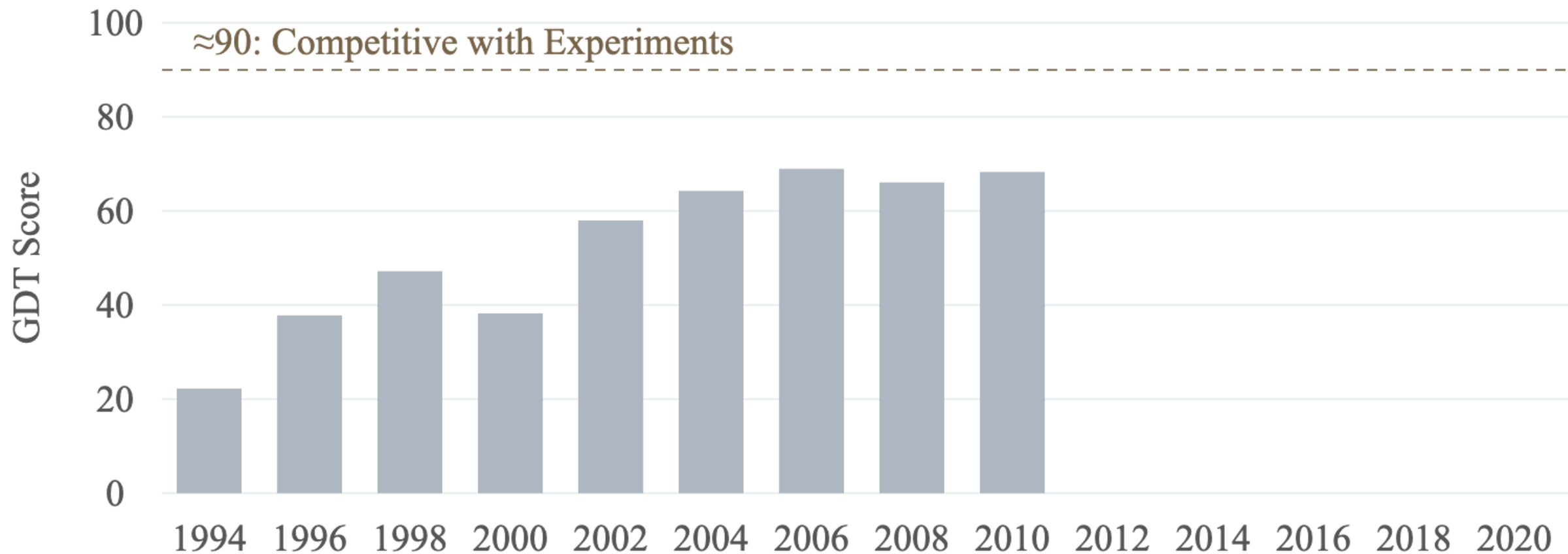
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

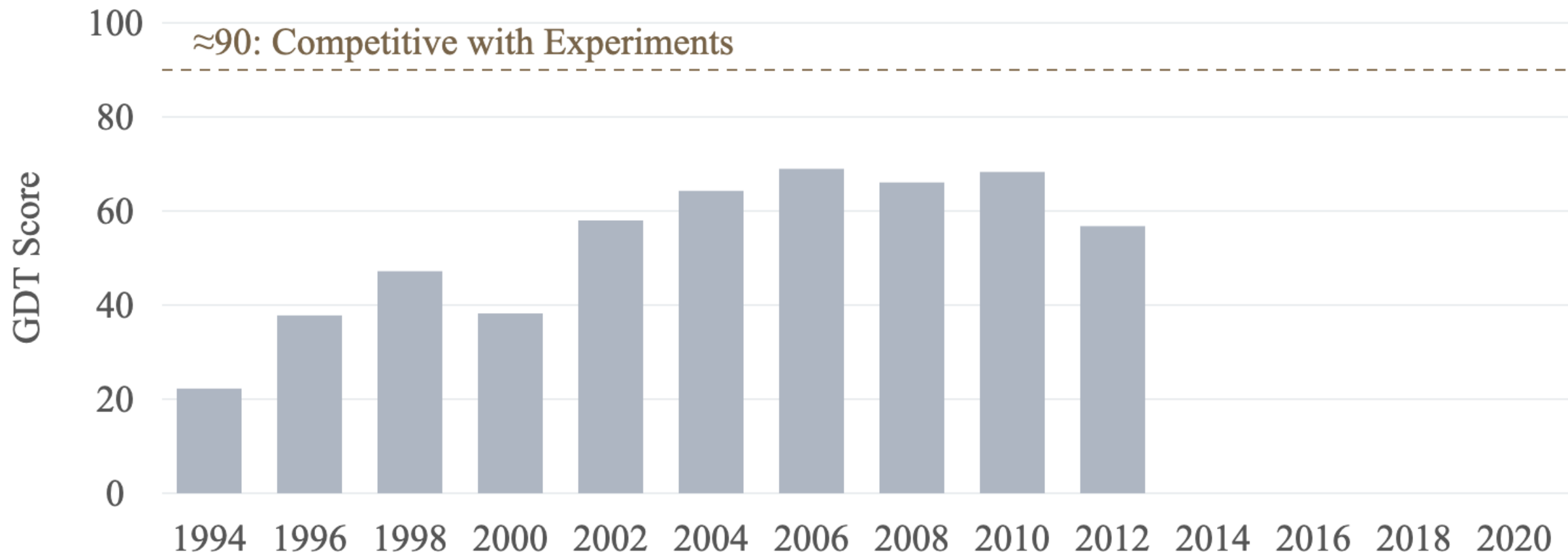
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

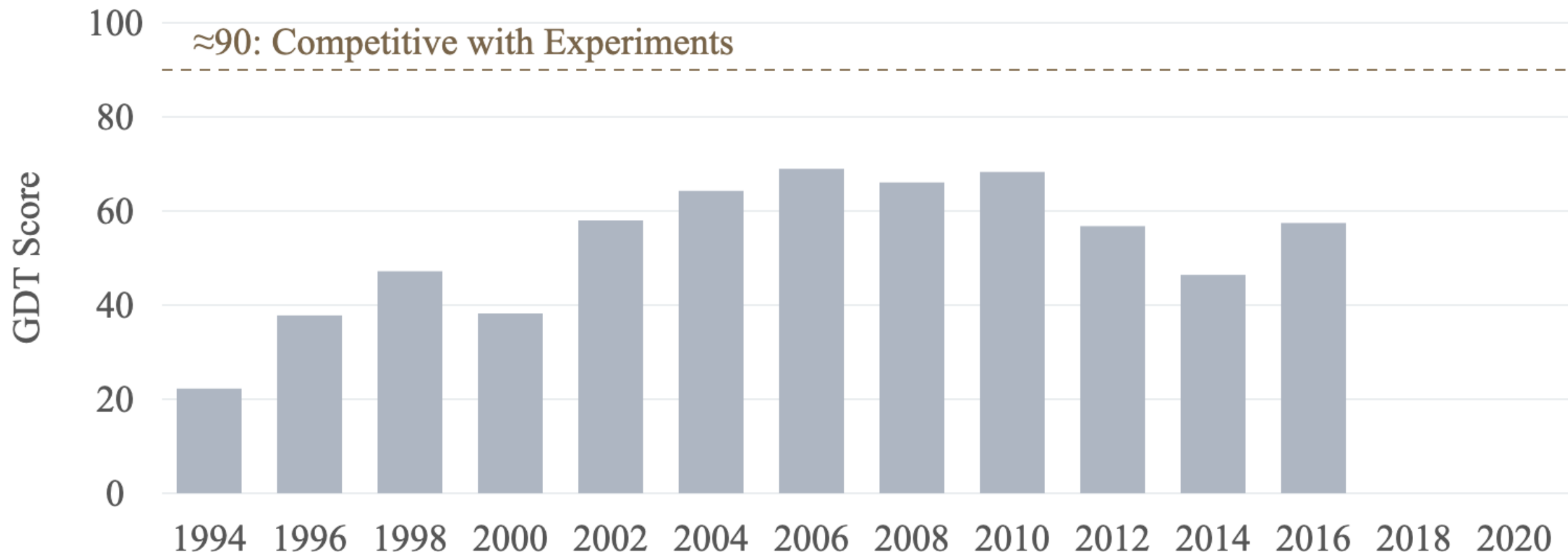
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

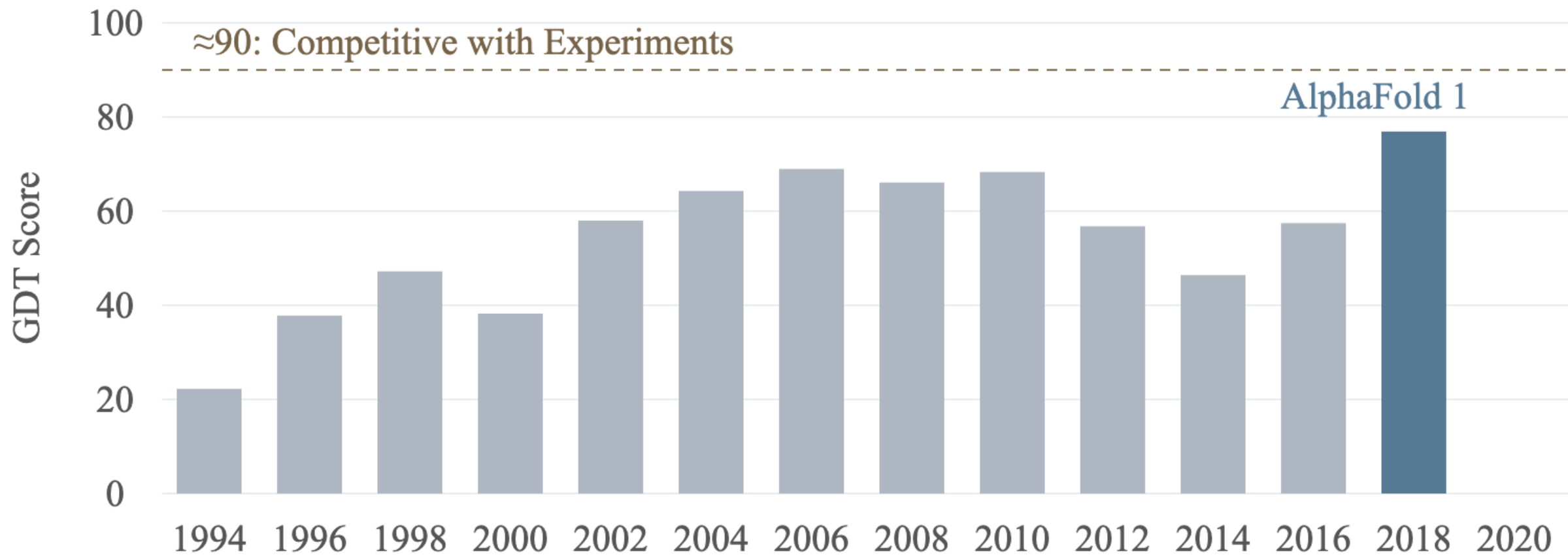
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

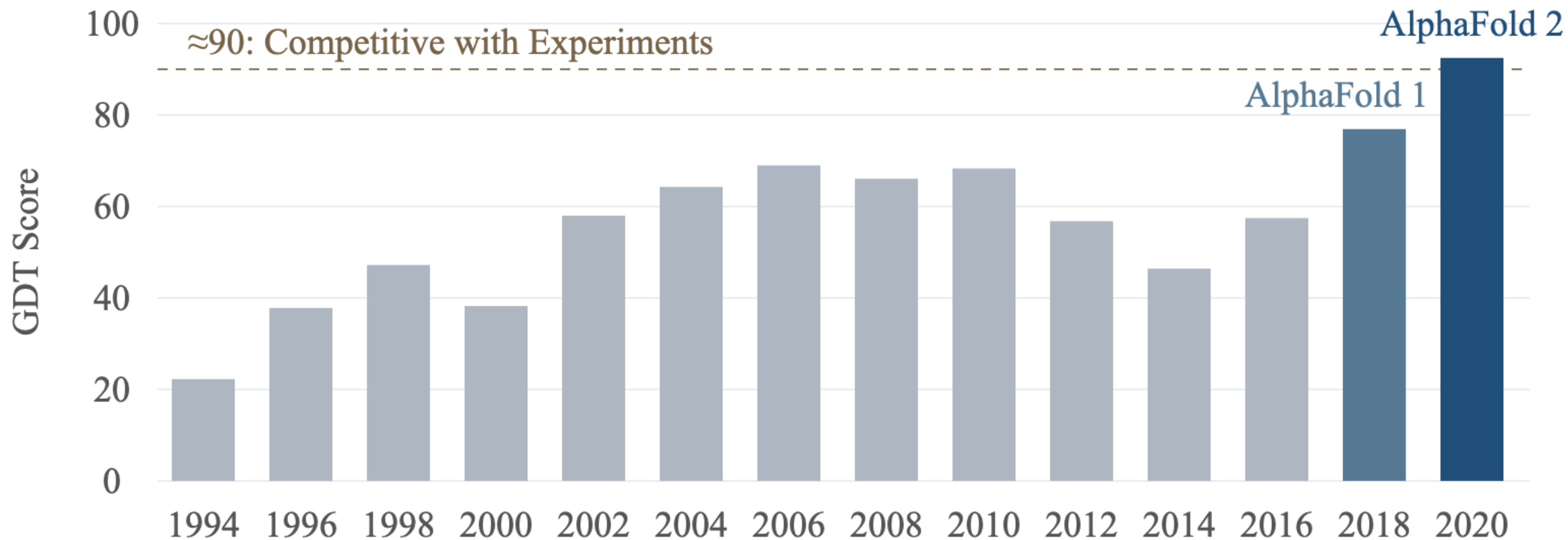
Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

CASP: Decades of Progress

Blind Assessment Since 1994



Median GDT Across Targets · Gebhart (2023)

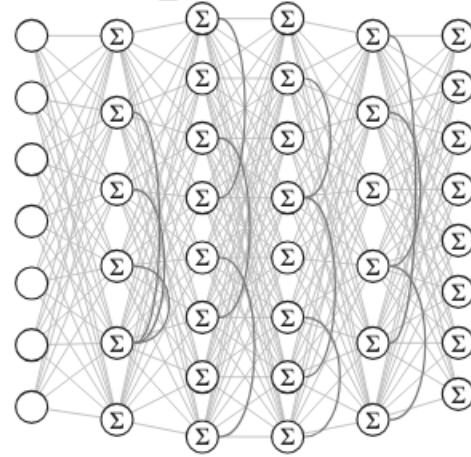
How AlphaFold Predicts Structure

Training: Learn from Solved Proteins

Amino-Acid Sequence

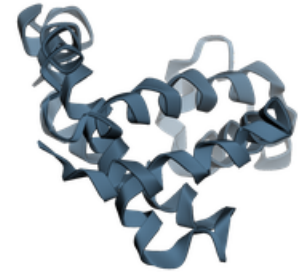


AlphaFold

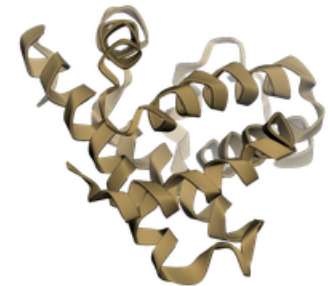



Learned Weights

Predicted Structure



Measured Structure



How AlphaFold Predicts Structure

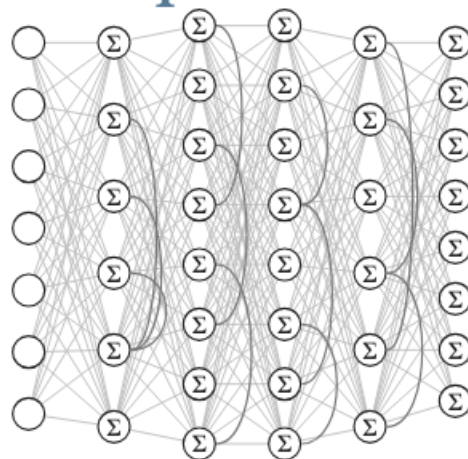
Training: Learn from Solved Proteins

Amino-Acid Sequence

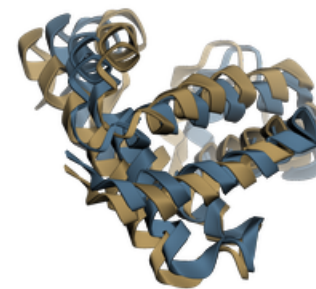
V L S E G E



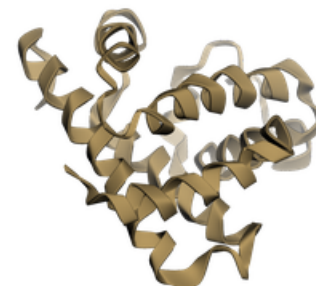
AlphaFold



Predicted Structure



Measured Structure



Learned Weights

Use Prediction Error to Adjust Weights

How AlphaFold Predicts Structure

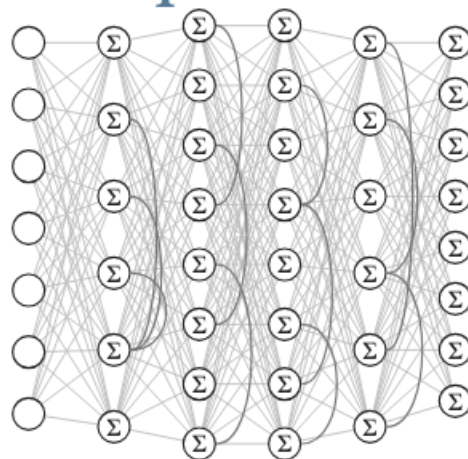
Inference: Predict a New Structure

Amino-Acid Sequence

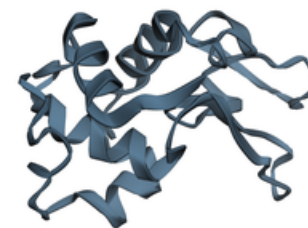
K V F E R C



AlphaFold



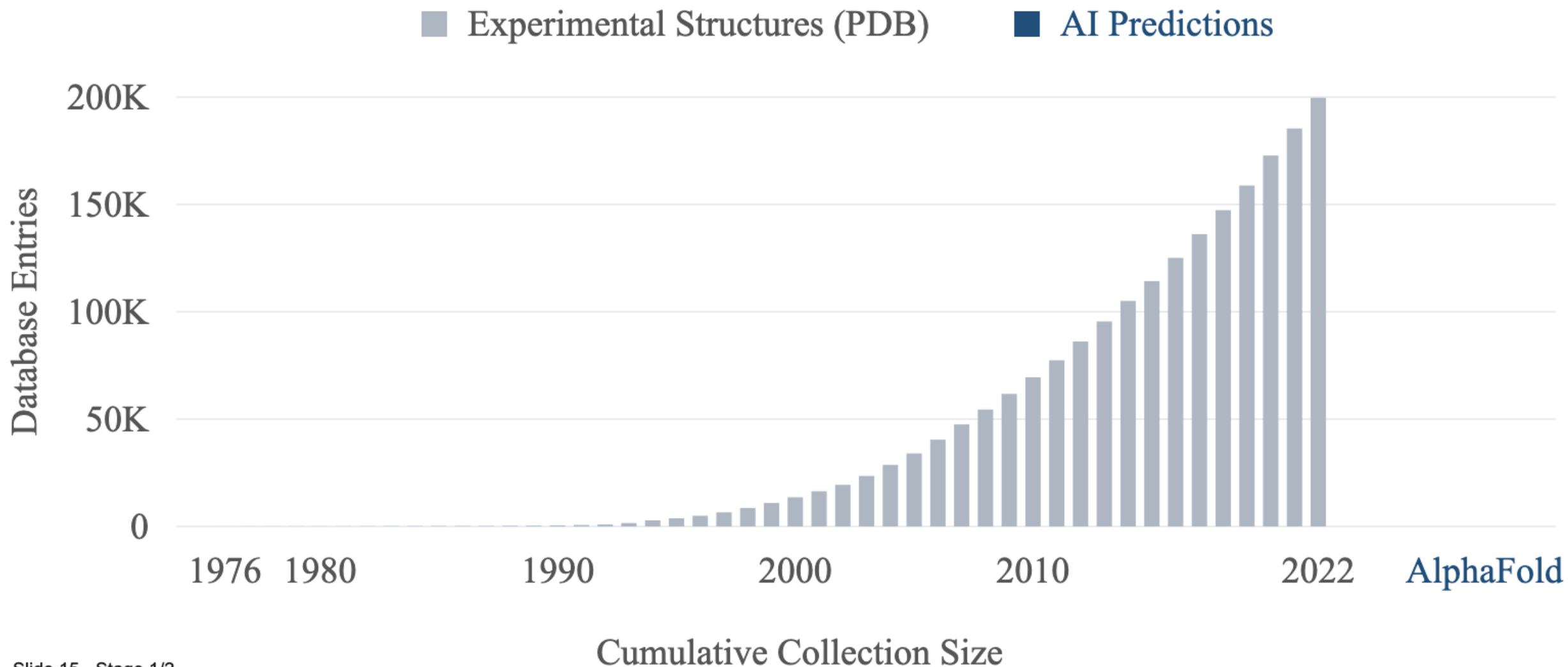
Predicted Structure



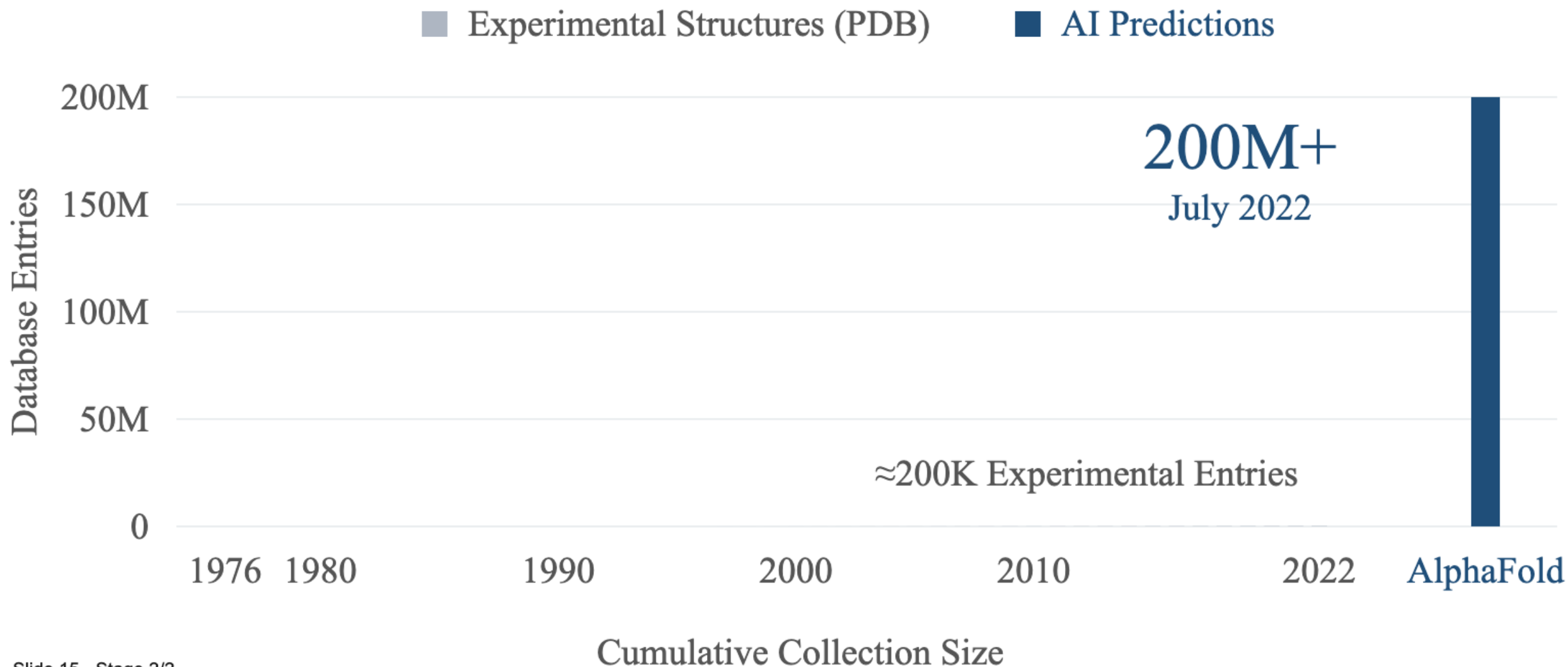
Learned Weights

New Input · Fixed Weights

Protein Structures at Scale



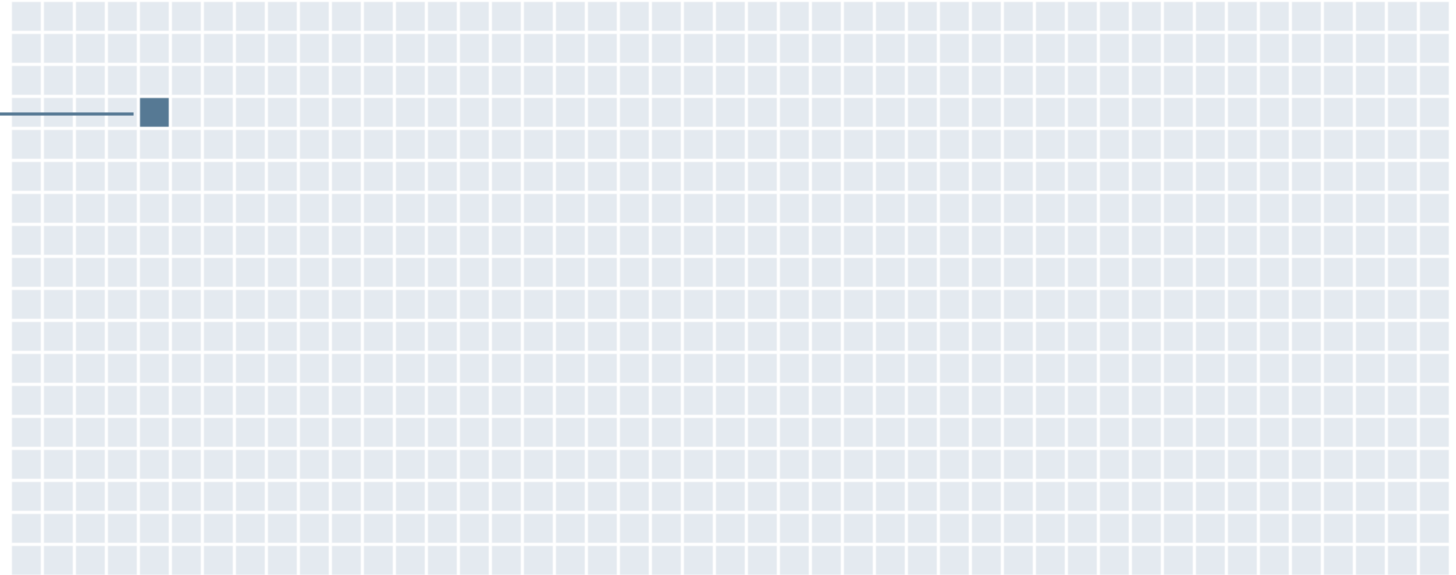
Protein Structures at Scale



From Evolution to AI Protein Design

Possible Amino-Acid Sequences

Natural
Proteins



AI Can Propose New Sequences for a Purpose

From Evolution to AI Protein Design

Natural Selection Favours Survival and Reproduction

Our Design Goal: Bind and Block a Snake Toxin

AI Proposes a Shape



Toxin Target

From Evolution to AI Protein Design

Natural Selection Favours Survival and Reproduction

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Toxin Target

Designed Protein

From Evolution to AI Protein Design

Natural Selection Favours Survival and Reproduction

Our Design Goal: Bind and Block a Snake Toxin

AI Proposes a Shape

AI Chooses a Sequence



Toxin Target

Designed Protein



Amino Acids for the New Shape

From Evolution to AI Protein Design

Natural Selection Favours Survival and Reproduction

Our Design Goal: Bind and Block a Snake Toxin

AI Proposes a Shape

AI Chooses a Sequence



G R I V V R ...

Amino Acids for the New Shape

Toxin Target

Designed Protein

AI Predicts Folding and Binding



Researchers Make and Test

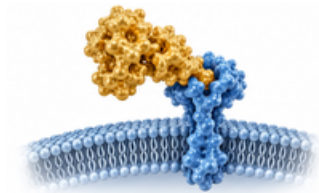
Applications of Protein Design



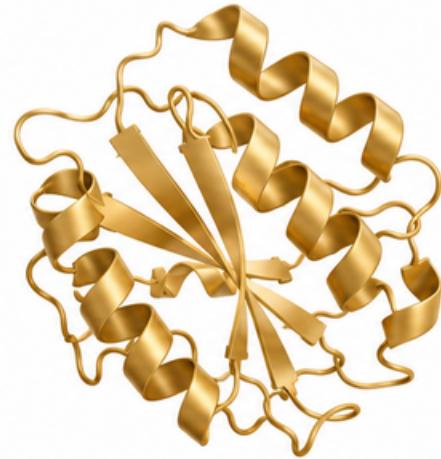
Antivenoms



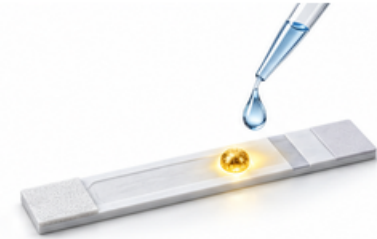
Vaccines



Targeted Medicines



Protein Design



Biosensors



Crop Protection



Recycling Enzymes

Research and Future Applications





David Baker

A group of men in tuxedos are standing on a stage. Two men in the center are highlighted with white labels and leader lines. The man on the left is wearing glasses and a light blue bow tie. The man on the right is bald, wearing glasses, a light blue bow tie, and a red sash with a medal. Other men in tuxedos are visible in the background and foreground.

David Baker

Demis Hassabis

A photograph of three men in tuxedos standing on a stage. The man on the left is David Baker, the man in the center is Demis Hassabis, and the man on the right is John M. Jumper. They are all wearing white shirts, white bow ties, and dark jackets. Demis Hassabis is also wearing a red sash. The background is dark, and other people in formal attire are visible in the background.

David Baker

Demis Hassabis

John M. Jumper

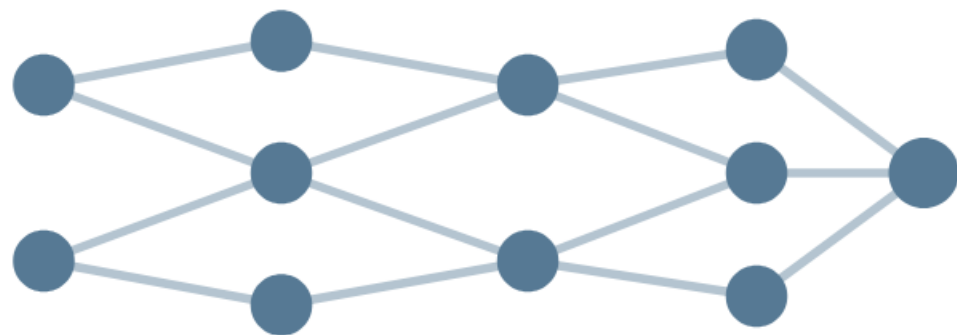
Who Is This?



Recall L1: The Deep Learning Breakthrough

L1, Slide 3 · From Biological Neurons to Modern AI

2012 · AlexNet



More Layers + Data + GPUs

Alex Krizhevsky · Ilya Sutskever · **Geoffrey Hinton**

AI Mathematics at Scale

OpenAI · October 2026

719

Manuscripts

372

Families of Results

Verification

Does the Argument Follow?

Understanding

Why Does It Work?

When Can We Use It?

Results at Different Verification Stages · Tuesday, 20 October 2026

AI Mathematics at Scale

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719

Manuscripts

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Families of Results

Verification

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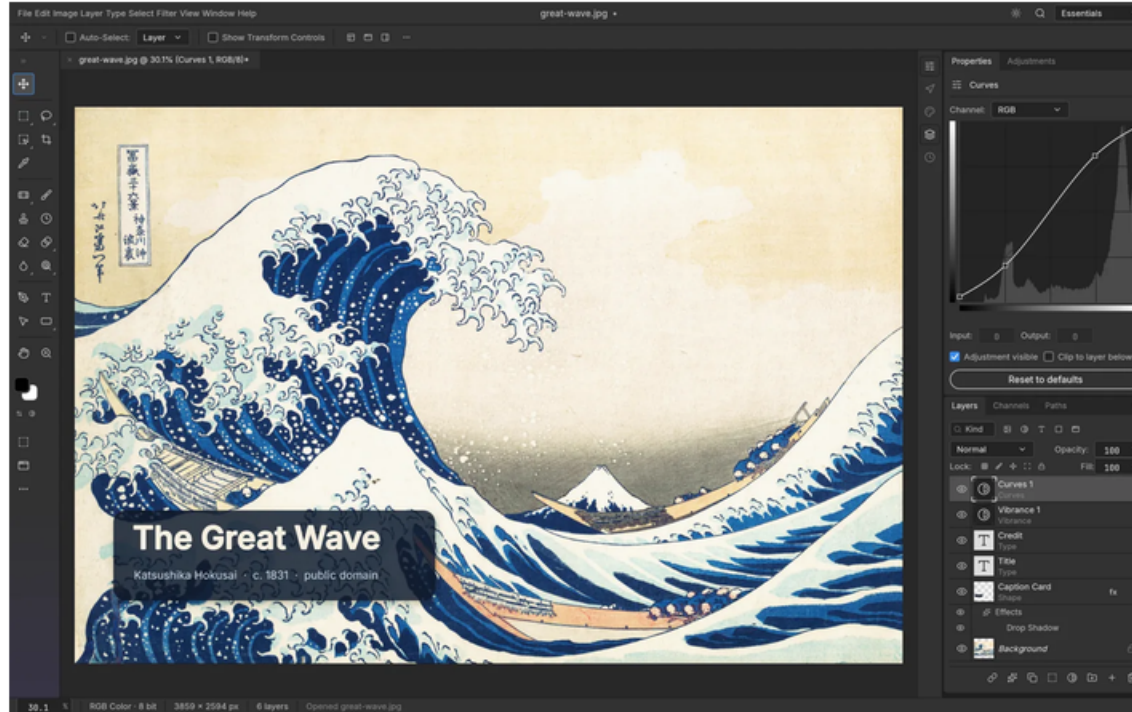
When Can We Use It?

Is a Correct Proof Enough?

Results at Different Verification Stages · Tuesday, 20 October 2026

AI-Built Software: Beyond the Demo

Selected Apps from ArtCraft's Creative Suite



What Would You Test?



PhotoCraft



VectorCraft



FilmCraft



LightCraft



EffectCraft

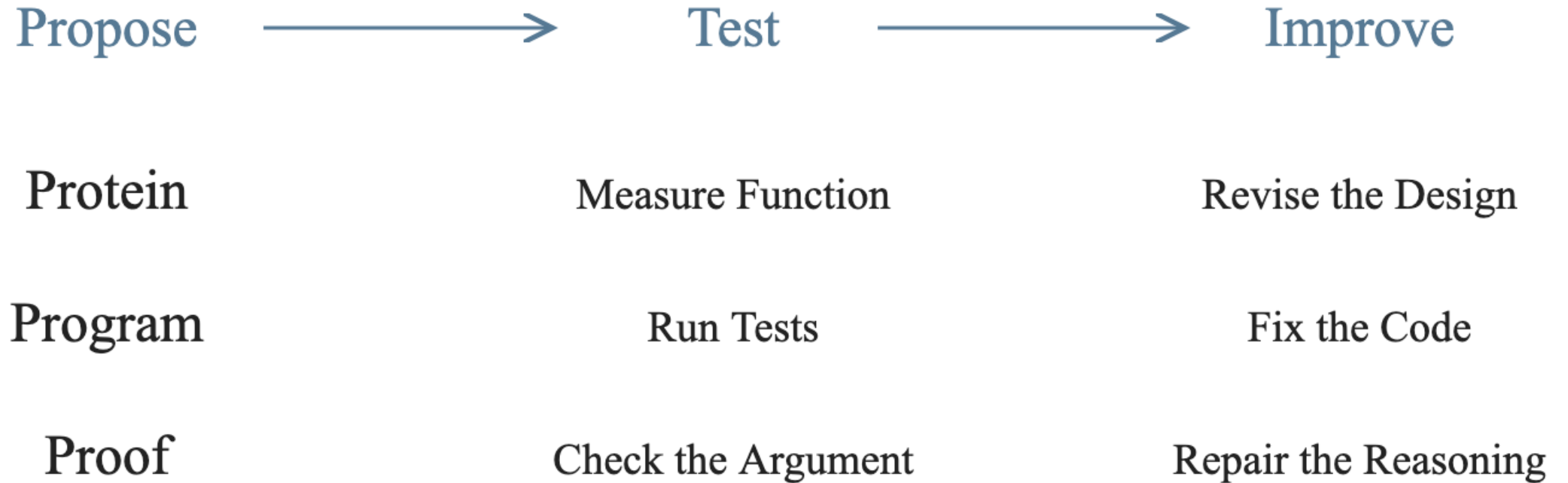


DesignCraft

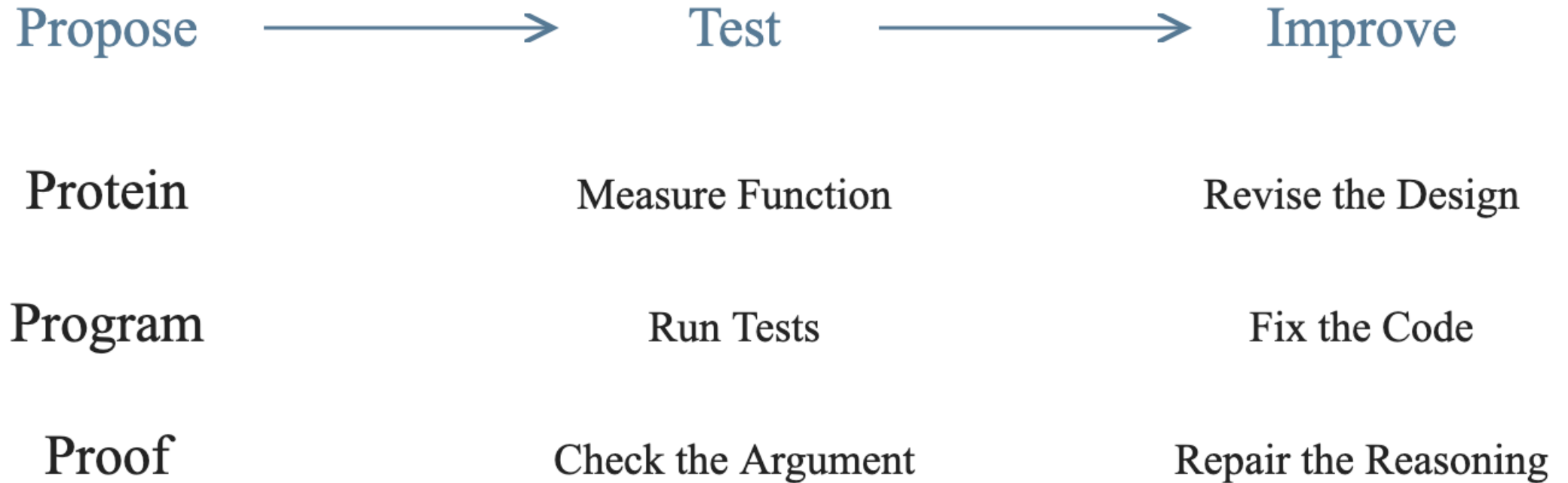


PdfCraft

When AI Can Test Its Ideas



When AI Can Test Its Ideas



How was it tested, and what hasn't been tested yet?



Exit Ticket: Discovery and Invention

Think of something you would like AI to help discover or invent in your daily life or field of study. Use the same example for all three answers.

1. What would you want AI to help discover or invent, and why would it be useful?
2. How would you test whether it works as intended?
3. Even if your discovery or invention works, who could be harmed or unfairly excluded? Suggest one way to address this.

Please reach out to a TA/STA if you encounter any technical problems before leaving.