# *HOW SCIENTISTS USE AI TO PREDICT PROTEIN SHAPES?*

*Biotech Buds*

St Leonard's Collage
Mason Gong
Grade 3, Lower Primary

## Introduction

Proteins are tiny machines inside all living things. They help our bodies move, grow, heal, and stay healthy. Every protein has a special 3D shape, and that shape decides what the protein can do. For example, insulin works like a key, and antibodies are shaped like a "Y" to catch germs.

Scientists wanted to understand protein shapes because they are important for making medicines and fighting diseases. But for many years, finding protein shapes was very slow and difficult.

Today, scientists use Artificial Intelligence (AI) called AlphaFold to predict protein shapes much faster. In 2024, the inventors of AlphaFold won the Nobel Prize in Chemistry. It was created by Google DeepMind and has changed biology and medicine forever.

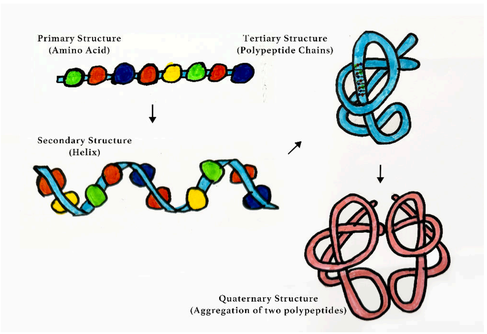
## Explanation of Scientific and Technical Principles

Proteins are made from long chains of amino acids. The chain folds itself into a special 3D shape. This is called "protein folding". (See Table 1) The shape of a protein is very important because it determines its function in the body. Scientists used to call this the "protein folding problem" because there are billions of possible shapes. A protein with 100 amino acids could fold in about $10^{50}$ different ways!

Before AI, scientists used experiments like X-ray crystallography, NMR, and Cryo-EM to study. These methods were expensive and could take months or even years. One scientist, Max Perutz, spent 22 years studying hemoglobin.

In 2020, AlphaFold achieved a major breakthrough in protein structure prediction. It is an AI system trained using thousands of experimentally determined protein structures. By analysing patterns between amino acid sequences and known protein shapes, AlphaFold learned how proteins are likely to fold. It uses deep learning neural networks to predict the relationships between amino acids and generate highly accurate 3D models. (See Table 2) Its predictions are often close to the accuracy of lab experiments, but can be produced in minutes instead of years.

**Table 1: How Protein Fold**





HEMOGLOBIN

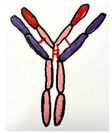
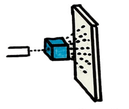

ANTIBODY

**Table 2: Traditional Protein Research Methods vs AlphaFold**

**Experimental Methods**


X-Ray Crystallography


Nuclear Magnetic Resonance


Cryo-Electron Microscopy

**AlphaFold**

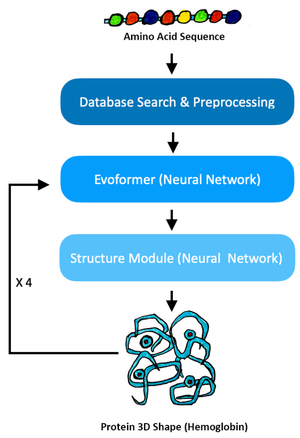



**Table 3: Before AlphaFold vs After AlphaFold**

| | BEFORE ALPHAFOLD | AFTER ALPHAFOLD |
|---|---|---|
| **Technology** | 🔬 Scientists used microscopes and laboratory experiments | 💻 Scientists use AI computers |
| **Time** | ⏳ Took months or years to find one protein shape | ⚡ Takes minutes to predict a protein shape |
| **Cost** | 💰 Very expensive equipment and laboratories | 🌍 Faster and cheaper for scientists worldwide |
| **Number of Protein Shapes Known** | 📉 About 170,000 known protein shapes in 50 years | 📈 More than 200 million predicted protein shapes |
| **Impact on Medicine** | 🦠 Slower research for medicines and vaccines | 💊 Faster development of medicines and vaccines |

## Significance and Impact

AlphaFold helps scientists design medicines faster and understand diseases better. By understanding protein shapes, scientists can study how viruses infect cells and develop new treatments and vaccines more quickly. During COVID-19, researchers used protein structure predictions to better understand the virus and support vaccine research.

Protein structure prediction can also help scientists create better food crops, design plastic-eating enzymes, and develop new ways to clean polluted water. Today, scientists have predicted more than 200 million protein shapes using AlphaFold. (See Table 3)

This discovery is important because it saves time and money, accelerates scientific research, and could help millions of people in the future.

## Acknowledgements

Thank you to my teacher, my family, and the scientists who created AlphaFold and shared their research with the world.

## References

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