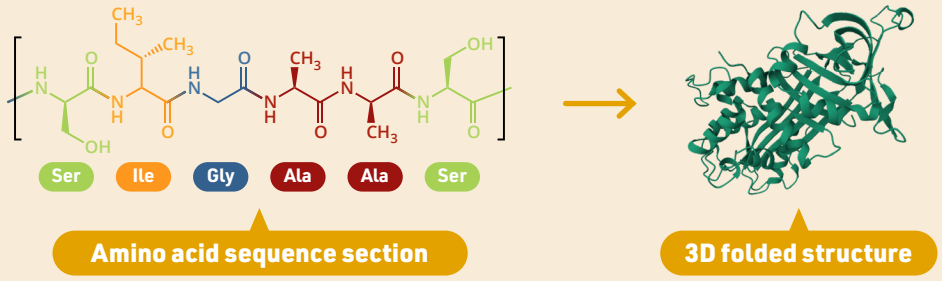
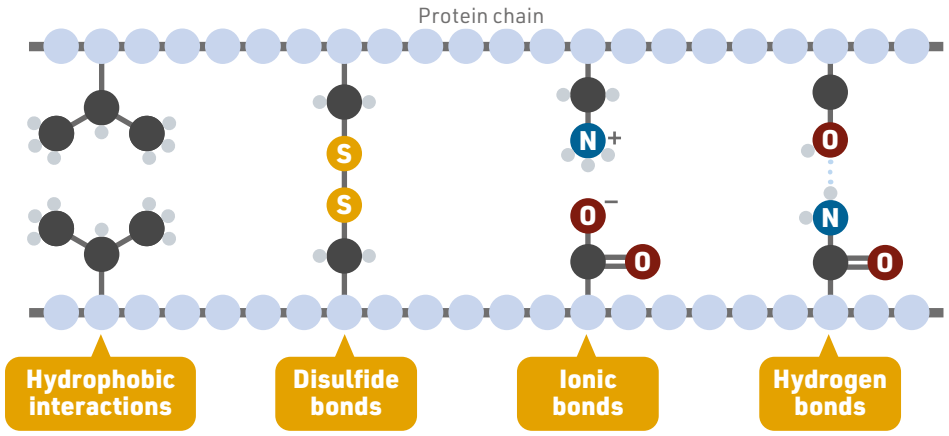
The 2024 Nobel Prize in Chemistry

The 2024 Nobel Prize in Chemistry was awarded to **David Baker** for computational protein design and to **Demis Hassabis** and **John M. Jumper** for protein structure prediction.

Proteins are important biological molecules formed from 20 naturally occurring amino acids. Proteins form folded 3D structures which are key to their function and properties, but the exact way in which they fold is hard to predict. A protein with just 100 amino acids could have 10^{47} different 3D structures.

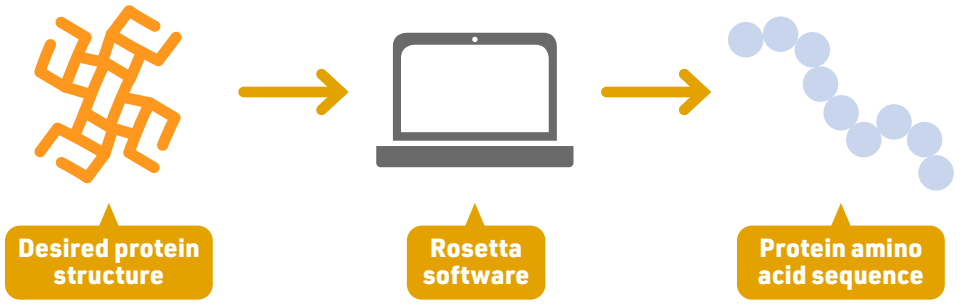


In 2020, **Demis Hassabis**, **John Jumper** and their co-workers unveiled an artificial intelligence model called AlphaFold2 to predict 3D folded structures of proteins. This is notoriously difficult because of the range of intermolecular forces in protein structures.



AlphaFold2 analyses amino acid sequences and evaluates how they might interact with each other. It has since been used to predict the structures of the almost 200 million known proteins.

David Baker developed Rosetta, software that also attempts to predict protein structures. He wondered if it was possible to work in the other direction: to start with a protein structure and use the software to work out its amino acid sequence.



Rosetta uses a database of protein structures and searches it for fragments with the same structure as the desired structure, pieces them together, then suggests an amino acid sequence based on this.

Baker's research group succeeded in doing this in 2003 to create an entirely new protein. They have since produced many other novel proteins that do not occur naturally.

WHY DOES THIS RESEARCH MATTER?

Being able to predict and design protein structures has benefits for the design of protein-based drugs, sensors, vaccines, catalysts, and more. It also aids our understanding of existing proteins and how they interact with other molecules.

Nobel Prize in Chemistry press release: https://www.nobelprize.org/prizes/chemistry/2024/press-release/