

How AI could supercharge the development of new drugs

Understanding the shapes of proteins is critical for advancing medicine, but until now, only a fraction of these have been worked out.

Researchers used a program called AlphaFold to predict the structures of 350,000 proteins belonging to humans and other organisms.

The instructions for making human proteins are contained in our genomes – the DNA contained in the nuclei of human cells.

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AlphaFold was able to make a confident prediction of the structural positions for 58% of the amino acids in the human proteome.

The positions of 35.7% were predicted with a very high degree of confidence – double the number confirmed by experiments.

Traditional techniques to work out protein structures include X-ray crystallography, cryogenic electron microscopy (Cryo-EM) and others. But none of these is easy to do: “It takes a huge amount of money and resources to do structures,” Prof John McGeehan, a structural biologist at the University of Portsmouth, told BBC News.

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Commenting on the predictions from AlphaFold, Prof McGeehan said: “It’s just the speed – the fact that it was taking us six months per structure and now it takes a couple of minutes. We couldn’t really have predicted that would happen so fast.”

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