FIVE QUESTIONS

ON THE USE OF ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL RESEARCH

FOR PETER NUSSBAUMER

Proteins consist of a chain of different amino acids, which can fold into complex three-dimensional structures. Based on the sequence of amino acids, Google subsidiary DeepMind's AlphaFold software is able to predict this 3D structure with high accuracy.

Mr. Nussbaumer, will this new software revolutionize the development of new drugs?

PETER NUSSBAUMER Without a doubt, this program represents a milestone in protein analysis. However, many different research disciplines contribute to the development of novel drugs. Of course, technical progress in one field benefits the entire development process, yet it is only one piece of the puzzle, so I'm not expecting a revolution.

How could AlphaFold advance the development of new drugs?

We could, for instance, use AlphaFold to obtain a new spatial structure of a protein involved in a specific disease. If it has a structural similarity to another protein whose function is already known, we could then potentially use that knowledge to infer the role of the disease-related protein. However, we also have to keep in mind what AlphaFold cannot do; for example, it can neither predict the ways in which proteins change over time, how their structure is affected upon binding to other proteins or drugs, nor the orientation of side chains. The software also does not tell us where and how a molecule binds to a protein, which is particularly crucial for the development of new drugs.

What is the current role of artificial intelligence in the development of new drugs?

Among other things, the answer to that depends on how one defines artificial intelligence. The computational power of modern computers, neural networks and machine learning have long been aiding us in pharmaceutical research. We also refer to this as "computational chemistry." Examples of this include making structural comparisons between known and unknown proteins or the use and evaluation of the vast amount of data generated during preclinical research. Computational chemistry is also extremely useful for interpreting gene activity patterns and predicting target proteins for drug development. Artificial intelligence will certainly become more important going forward, but we shouldn't expect miracles from it.

Will the LDC be using AlphaFold?

I don't know whether DeepMind will make the software available to us and at what price, but, at this point, I suspect that the costs would exceed the benefits to us. Perhaps the algorithm may be made public, thus becoming "open source" software.

Do you think that DeepMind may move into drug development?

I'm not privy to Google's plans, but, as I said, there's more to developing new drugs than a sophisticated program for the 3D analysis of proteins. Even so, I wouldn't provide our data to the company. In my view, the question at this moment is more about whether DeepMind will eventually offer structural analysis as a paid service. So far, research groups have provided free access to the structural data from their studies.

Interview: Harald Rösch

Peter Nussbaumer is Managing Director of the Lead Discovery Center in Dortmund (LDC), which is a spin-off of Max Planck Innovation; LDC is dedicated to the development of new drugs.

ILLUSTRATION: SOPHIE KETTERER FOR MPG