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China's Zelixir Biotech predicts monkeypox protein structures for drug discovery

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Publishes 600+ protein structure predictions for the Monkeypox proteome



Zelixir Biotech, based in China, has predicted more than 600 structures and added functional annotations of proteins from monkeypox virus proteomes amid the recent emergence of monkeypox cases in Europe and the United States.

The predicted structures are expected to help experts worldwide to develop structure-based drug design and monkeypox vaccines.

The predicted protein structures are AI-generated by AlphaFold2-Batch (originated from the DeepMind AlphaFold2), the company's self-developed MPI-based structure prediction pipeline with heterogeneous parallelism powered by supercomputing infrastructures.

AlphaFold2-Batch, which is available on the company's platform "ZCloud", has largely boosted both the efficiency and the precision of the predictions by nearly two orders of magnitude acceleration compared to the original AlphaFold2 pipeline, generating results without any compromise of accuracies.

"We hope our work can accelerate the development of monkeypox vaccines and drug discovery. We will keep updating and publishing our new research findings as our research progresses." said Dr Sheng Wang, CEO, Zelixir Biotech.