Huawei Cloud's Pangu drug molecule model accelerates new drug discovery

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In the pharmaceutical industry, an average of over $ 1 billion and 10 years is needed to put a new drug on the market, from development to approval

On September 19, HUAWEI CONNECT 2022 kicked off in Bangkok, Thailand. At the event, Ken Hu, Rotating and Acting Chairman of Huawei, delivered a keynote titled "Unleash Digital", and spoke about how the First Affiliated Hospital of the Medical School at Xi'an Jiaotong University used artificial intelligence (AI) to expedite pharmaceutical R&D and new drug discovery.

By using an AI-aided drug design service powered by China-based Huawei Cloud's Pangu Drug Molecule Model, Professor Liu Bing of the First Affiliated Hospital of the Medical School at Xi'an Jiaotong University and his team developed a new broad-spectrum antimicrobial drug in just one month, and R&D costs were slashed by 70%.

A major challenge in new drug discovery lies in the screening of hundreds of millions of existing drug molecules. Traditionally, drug screening was performed by experts in labs, which was costly, slow, and had a high failure rate.

The Huawei Cloud Pangu Drug Molecule Model has been trained using the data of 1.7 billion drug-life molecules, and can predict the physicochemical properties of drug compounds and score them based on their druglikeness. Researchers can then do targeted experiments to verify drug compounds that have the highest scores.

Moreover, the Pangu Drug Molecule Model's molecular structure optimizer can be used to optimize the structure of lead compounds, minimizing the potential side effects of the new drugs on normal human cells.