



NEONIOUS

PRESS RELEASE

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Neonious Biotech is pioneering a new approach for in silico drug analysis for safety and side effects, reducing cost risks in drug development and reducing animal testing and humans harmed in trials. Anyone can help the mission by running needed simulations for this service on their computers, earning money paid in cryptocurrency along the way.

Drug development harms animals and humans, and cost a lot of money

After finding a potential drug to treat a disease, preclinical studies are done with the goal of understanding whether the discovered drug might be harmful for humans. This very often involves testing the drug on animals. Then, the human trials start, which in the early phases of the trials usually have the goal of assessing safety and side effects further.

In the 1960s, for a few years, the drug Thalidomide was sold under the brand name Contergan as a medication to treat anxiety, trouble sleeping and other conditions. It was taken off the market when it was discovered that this drug, taken by pregnant women, was responsible for babies being born with severe deformities. More than 10,000 babies were affected.

What if Contergan was being developed today? With today's standards, the shocking effects of the drug most probably would be discovered in the human trials. To discover this, at least one baby would be harmed and born disabled.

However, we do not need to concentrate on this drastic example to see the problems associated with drug development: Most potential drugs do not reach the human trials. 2/3 of all drugs which reach human trials, fail the trials in the first two phases, when safety and side effects are still being questioned. There is not only an immense cost associated with these failures, many animals and also humans in the trials are harmed in the process.

Neonious Biotech's service reduces risks

After three years of development, Neonious Biotech is now offering to analyze drugs in development for safety and side effects, for drugs in the early steps of preclinical studies or latest in human trials. To get this done, Neonious Biotech is utilizing a novel automated screening pipeline.

The pipeline begins with docking simulations, just as done with in silico drug discovery, with the exception that not many simulations are done with many potential drugs and one target protein, but rather many simulations of a drug with most of the catalogized proteins of the Protein Data Bank archive. For this, where applicable the catalogized proteins are first transformed by Neonious Biotech into various confirmations by running many MD

simulations. In some cases, the docking simulation results are then verified with additional MD simulations.

After this step, Neonious' research team analyzes the simulation results for safety and side effects. Also, the team runs additional simulations or do lab tests where needed. At the end of the process, a detailed report is written and presented to the customer.

With this service, the effects of Contergan (Thalidomide) would have been discovered early, before harming anyone, as the growth factor protein which Thalidomide binds to is one of the proteins catalogized in the Protein Data Bank. Also, the costs associated with the human trials would have been avoided.

Last, the service helps to visualize the reason for side effects, allowing potential drugs to be optimized for less side effects instead of simply being discarded. Promising drugs which were already discarded because of side effects can also be analyzed by Neonious, to potentially put them back into the process.

Simulations can be done cost-effective on the distributed Neonious Network

Pharmaceutical companies interested in the service can choose between Neonious running the needed simulations on private clusters or Neonious running them on the far more inexpensive Neonious Network.

The Neonious Network consists of computers of consumers, which run Neonious' simulation software. For running the software which does the calculations and/or validates calculations done by others, the owners of these computers get paid with Neonious' own cryptocurrency, the Neonious Token (MDSIM).

This allows Neonious Biotech to run the simulations at 30 % of the normal computing costs. For the owners of these computers, this still amounts to 2.5x of what they can earn with using the same computer to mine cryptocurrency.

The first full analysis of a drug for safety and side effects is already scheduled for August 2021 on the Neonious Network. People interested in helping out with the simulations can visit <https://www.neonious.org/en/RunNode> for more information.

Contact Info

Neonious GmbH
Münsterstr. 246
40470 Düsseldorf

CEO
Thomas Rogg

Web: www.neonious.org
Fax: +49 211 9241 8172

Mail: t.rogg@neonious.org
Tel.: +49 211 9241 8187