SIMULATING DRUGS TO ELIMINATE DISEASE

Molecular drug actions are a black box – understanding a drug's behaviour is usually based on experimental results rather than physical understanding. As an example, while lithium compounds are known to help alleviate the symptoms of bipolar depression, the actual mechanism by which they assist brain chemistry is poorly understood. This leaves scientists to piece together a picture of how a drug interacts with a patient through a variety of experiments.

There are many reasons for our inability to understand a drug's interactions at the molecular level, including the impossibility of examining these processes in live patients, the incredible difficulty of seeing drug molecules act on a sub-microscopic scale, and the extreme speed at which chemical interactions occur. This incomplete picture of drug interactions leads to very lengthy drug discovery processes, leaves unfortunate side-effects hidden until experimental trials, and makes some types of valuable experiments completely impractical.

DIGITAL DRUGS

That's why computational biophysical chemists at Memorial University of Newfoundland have created computer models of biological systems that can simulate drug activity at the molecular level. By moving molecule interaction into the digital realm, researchers can do things that are impossible to observe in the real world. They are able to simulate any biological chemical process, such as how drugs are absorbed through cell walls and other membranes, and create frame-by-frame visualizations of these processes, no matter how fast, rare, or tricky they are to capture.

As might be expected, there are significant computational resources needed to perform and store each simulation containing the precise atomic-scale motion of millions of molecules at extremely rapid timescales. That's why Memorial researchers are using the resources of ACORN-NL to help. ACORN-NL is the Newfoundland partner of the National Research and Education Network (NREN) that, with NREN partners, provides high-speed networking access to Canada's higher education facilities. Through ACORN-NL, Memorial scientists can run their simulation remotely on Compute Canada's cloud-computing resources, allowing them to take advantage of more powerful hardware and to scale their compute power as needed. The ACORN-NL network is necessary for analysis too, allowing transfer of massive simulation data sets and virtual movies of the atomic interactions between researchers' local machines and the cloud.

WHAT IS THE NREN?

The National Research and Education Network (NREN) is an essential collective of infrastructure, tools and people that bolsters Canadian leadership in research, education, and innovation. CANARIE and its twelve provincial and territorial partners form Canada's NREN. We connect Canada's researchers, educators, and innovators to each other and to data, technology, and colleagues around the world.

VIRTUAL LABORATORY POWER

Molecular simulations allow scientists to understand which physical features of a drug molecule's construction allow it to function within the human body. They can be used to model the interactions of drugs in all the ways they interact with the body including their passage from the stomach, across the cell membrane, and into their target. They make it significantly easier, faster, and less expensive to screen millions of possible compounds to isolate potential drugs for a specialized application, letting researchers focus on a handful of promising drugs identified through simulation rather than the enormously expensive alternative of testing them all by hand.
The ever-watchful computer can also reliably identify extremely rare events occurring within simulations, making it possible to capture sporadic but critically important events for study. Researchers are then able to develop new algorithms to focus simulations on these rare events, which often have big consequences.

These capabilities enabled by simulation help researchers fashion new drugs that are more effective or easier to fabricate, predict the behavior of existing drugs for new applications, and tailor-edit drugs to reduce their unwanted side effects – things that are necessary for improving the quality of life for every-day Canadians as well as humanity in general. As scientists around the world search for better drugs in an effort to eliminate human disease, they rely on Canadian contributions to computational biophysics to help them get there. And those biophysicists in turn rely on ACORN-NL and Canada's NREN.

For more information, visit:

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