Tens of thousands of new tricks for existing drugs

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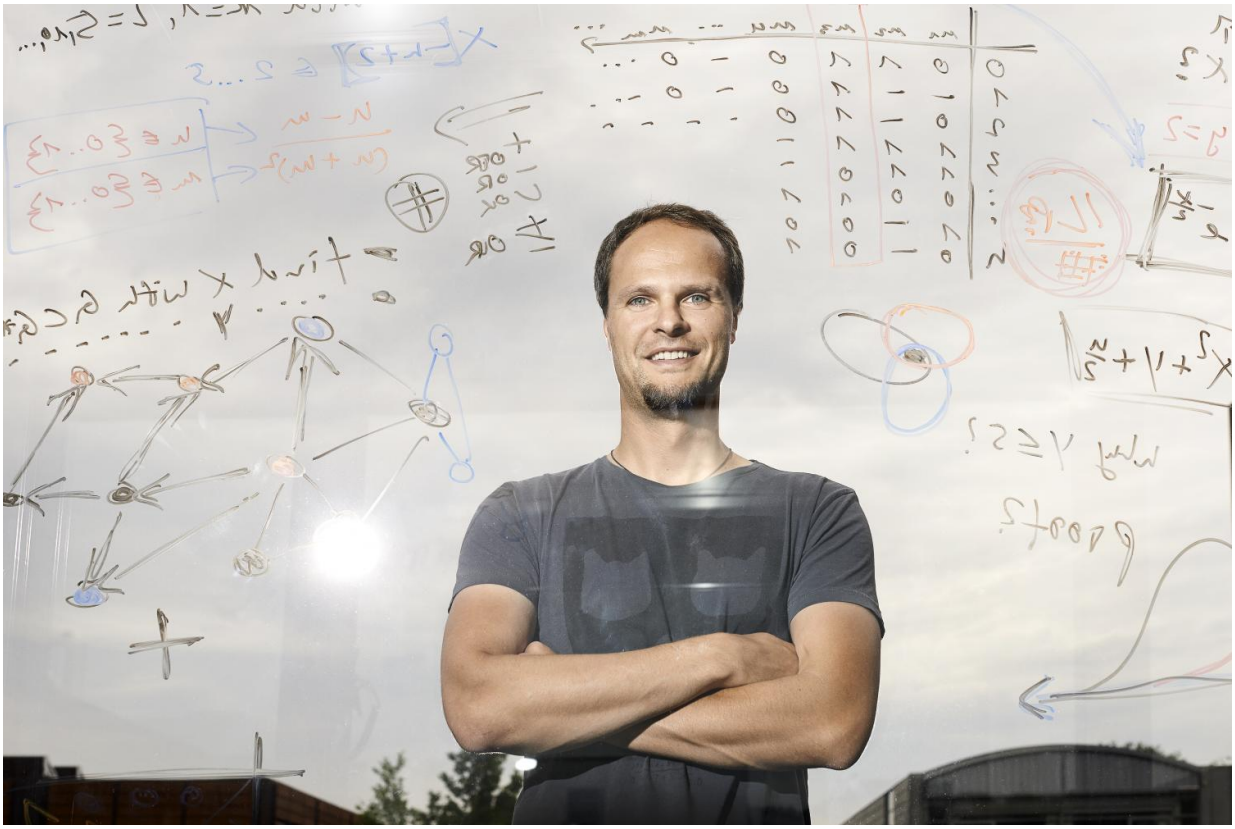

Dr. Jan Baumbach, University of Southern Denmark. Credit: University of Southern Denmark

One drug, one disease. This is how we traditionally think about pharmaceutical drugs, but many of them are actually effective for more

than one disease.

Take the drug gabapentin, originally developed for treating epilepsia, but today commonly prescribed as a pain killer. Or sildenafil, originally developed for treating high blood pressure, but today more often used to treat erectile dysfunction.

Value for patients

"With our recent research we predicted yet unknown beneficial effects for many drugs - on different diseases than they were initially developed for. This is of immense value, both for patients and for the pharmaceutical industry - in particular when it comes to avoiding expensive clinical trials on drug safety", says associate professor Jan Baumbach, University of Southern Denmark.

Jan Baumbach is an expert in computational biomedicine and his research focuses on retrieving meaningful information from big data generated nowadays in the health care sector.

Together with his colleagues Peng Sun from the Max-Planck Institute for Informatics in Germany, Jiong Guo from ShanDong University in China, and Rainer Winnenburg from Stanford University in the U.S., Baumbach has used novel big data analytics methods to trawl through massive pharmaceutical data, looking for drugs having a high potential to be what the scientists call "repurposable".

The results are published in the journal *Drug Discovery Today*.

From inflammatory diseases to Parkinson's

Baumbach's team found ca. thirty thousand "repurposable" drug

candidates. Of these ca. eleven thousand have already been mentioned in scientific literature, and about 1,400 are reported in literature as concrete "repurposing" options.

This leaves roughly 19,000 highly confident drug-disease combinations that no one has yet considered to investigate - a huge gold mine for future pharmaceutical research.

One example is prednisone, originally developed to treat inflammatory diseases. This drug turns out to hold promise for treating Parkinson's disease as well. Another example is chlorpromazine, originally developed to treat schizophrenia, but likely to be effective against tuberculosis as well.

Avoiding animal trials

According to Baumbach and his co-authors, the pharmaceutical industry is facing great challenges due to a decreasing speed of new drug discoveries. New approaches are necessary.

"Drug design is extremely expensive, time-consuming and becoming increasingly complicated. Our approach is a way of inferring new purposes of existing drugs computationally - saving a lot of time, money and maybe more important, avoiding potentially dangerous animal and clinical trials", says Baumbach.

In their paper, the researchers write that the development cycle can be reduced through repositioning by as long as five years, compared to traditional drug discovery pipelines, adding:

Reduced safety risk for patients

"Repurposable drugs have significantly reduced safety risks for patients, because already known and registered drugs have been thoroughly studied with respect to their toxicity and possible side-effects."

The total list of the discovered 31,731 candidates is freely available and can be obtained from the researchers or the publication's online supplementary material.The list includes, for instance, a drug used to treat hypertension or one with anti-inflammatory effect given after organ transplantation that might be well suitable for treating certain cancer types.

Side bar: How did they find the candidates?

Computational approaches play an increasingly important part in nowadays pharmaceutical discoveries. In this case, the researchers created a new data model allowing them to mine for shared properties between genes, drugs and diseases, and to combine this novel data structure with an artificial intelligence to mine millions of scientific publications for approving or disproving hints.

Provided by University of Southern Denmark