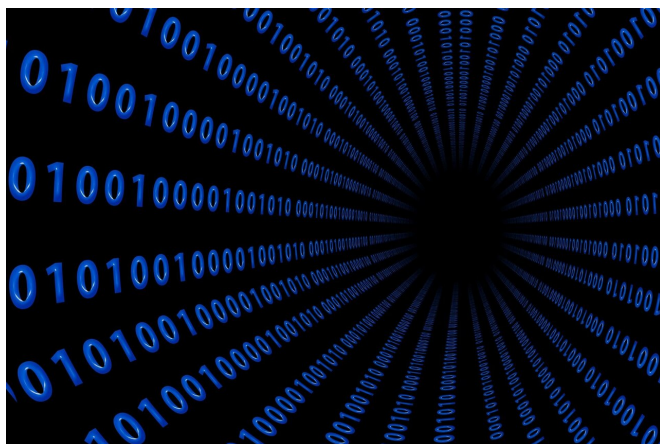


New database could accelerate drug repurposing for various diseases

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Credit: Pixabay/CC0 Public Domain

Researchers have created a new open-access database of information on drug candidates and how they are metabolized by the body, which could help speed up the repurposing of old drugs as new treatments.

There is an urgent need for more effective treatments for many conditions, including COVID-19, cancer and malaria. But the process of developing new drugs is costly, can take decades, and often leads to failed treatments. The [database](#), called NICEdrug.ch and described today in eLife, may help expedite the process by helping scientists find promising, existing drugs that might be repurposed for these diseases.

"By finding a way to improve how we discover and design [new drugs](#), we could reduce the time and costs involved in the drug-development process," says lead author Homa Mohammadi Peyhani, Postdoctoral Researcher at the Laboratory of Computational Systems Biotechnology, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland.

To help, Peyhani and colleagues created the NICEdrug.ch database with information on 250,000 potential drug molecules. The database includes detailed analysis of the drugs' structures, the enzymes they target, how they are likely to be altered by human metabolism, and their potential side effects.

Using their database, the team showed that it could accurately predict the behavior of drug-enzyme pairs around 70% of the time, and that it was 100% accurate for half of the pairs tested.

They then used the system to look for drugs that could be repurposed for cancer, high cholesterol, malaria and COVID-19. Their search yielded some clues on how scientists might alleviate the toxic side effects of the cancer drug 5-fluorouracil. They also identified shikimate 3-phosphate as a potential [drug](#) to treat the liver stage of malaria with fewer side effects. And they identified over 1,300 potential anti-COVID-19 drugs, including some that are already safely used to treat a number of other conditions. Further studies are now necessary to validate that these drugs can be repurposed for this disease.

The researchers have made the NICEdrug.ch database available for others as an open-access resource. In addition to helping find new purposes for existing drugs, the system may help scientists understand why some drugs cause harmful side effects and either identify ways to alleviate them or explore alternative drugs.

"Our hope is that scientists and [decision makers](#) in the [pharmaceutical industry](#) alike can use this unique database to better inform their research and clinical decisions—saving time, money and ultimately lives," concludes senior author Vassily Hatzimanikatis, Associate Professor of Chemical Engineering and Bioengineering at EPFL.

Details of the database were published in the

journal *eLife*.

More information: Homa MohammadiPeyhani et al, NICEdrug.ch, a workflow for rational drug design and systems-level analysis of drug metabolism, *eLife* (2021). DOI: [10.7554/eLife.65543](https://doi.org/10.7554/eLife.65543)

Database: [NICEdrug.ch](https://www.nicedrug.ch/)

Provided by eLife

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