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Researchers are on their way to predicting what side effects you'll experience from a drug

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Researchers at the University of California, San Diego have developed a model that could be used to predict a drug's side effects on different patients. The proof of concept study is aimed at determining how different individuals will respond to a drug treatment and could help assess whether a drug is suitable for a particular patient based on measurements taken from the patient's blood.

"We're not just interested in predicting the efficacy of a drug, but its side effects as well," said Bernhard Palsson, the Galetti Professor of Bioengineering at the Jacobs School of Engineering at UC San Diego. "Side effects are very personalized. Two different people can take the same drug, but one person might experience side effects while the other doesn't." Palsson and his team published their new study on Oct. 28 in the journal *Cell Systems*.

"There needs to be a good way to obtain data about a drug's side effects before exposing a lot of people to the drug. This predictive model could be used to figure out what these side effects are ahead of time," said UC San Diego alumnus Aarash Bordbar, who did this research while a Ph.D. student in Palsson's Systems Biology Research Group.

Researchers said that this predictive model would be extremely useful for pharmaceutical companies during the drug development stage. For example, pharmaceutical companies could conduct predictive screenings

for drugs before clinical trials and determine which groups of patients would experience side effects and which ones wouldn't.

The model predicts how variations in different people's genes impact how they metabolize a drug. Researchers used data from different people's genotypes and metabolism to build personalized models that simulate how a drug will affect a particular set of cells in the body.

"This is a unique approach to obtain personalized, predictive and mechanistic descriptions of people's physiology based on their genetic and metabolic makeup," said Palsson.

In this study, researchers focused on modeling drug side effects on red blood cells. Palsson and his team were interested in red blood cells because they are the simplest human cells and are readily available from blood samples. Also, the red blood cell provides a simple platform for researchers to find health markers that are related to a drug's side effects.

The study was based on genomic and metabolomics data obtained from blood samples of 24 individuals. Researchers used these data to build a personalized, predictive model for each individual. Researchers then used these predictive models to understand—at the metabolic level—why some individuals experienced side effects to ribavirin, a drug used to treat hepatitis C, while other individuals did not. A side effect of ribavirin is that it causes anemia—a condition characterized by a decrease in red blood cell levels—in approximately 8 to 10 percent of patients.

"A goal of our predictive model is to pinpoint specific regions in the red blood cell that might increase susceptibility to this side effect and predict what will potentially happen to any particular patient on this drug over time," said Bordbar.

The model is still at a proof of concept stage, and researchers said that they'd need to study a much larger sample size—hundreds of people, rather than dozens—to see how their model's predictive capabilities hold up.

"This study is a step forward in demonstrating that patients could be precisely treated based on their genetic makeup," said Palsson.

As a next step, researchers are also looking to develop predictive models for platelet cells, which are more complex than red blood cells. The ultimate goal is a liver cell model, researchers said, because the liver is where the majority of drugs are metabolized and where many drug side effects are manifested.

More information: "Personalized Whole-Cell Kinetic Models of Metabolism for Discovery in Genomics and Pharmacodynamics," by Aarash Bordbar, Douglas McCloskey, Daniel C. Zielinski, Nikolaus Sonnenschein, Neema Jamshidi, and Bernhard O. Palsson. The paper was published Oct. 28, 2015 in the journal *Cell Systems*. www.cell.com/cell-systems/pdf/ … -4712(15)00149-0.pdf

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