

BHSAI Scientists Work to Predict Adverse Drug-Drug Interactions

Prescription drugs and medications are safe when we take them as directed. However, once we start taking more than one type of drug, our risk of experiencing adverse health reactions due to the combination increases. Although we now have over 1,000 drugs approved by the Food and Drug Administration (FDA), most drug combinations are never evaluated for safety. If certain drug combinations have the capacity to affect our health, we need to be able to flag them.

Given the large number of commercial drugs, it is not practical to perform clinical safety evaluations for all combinations. This is why we typically only become aware of such effects from incidents reported after the drugs have reached the market. Scientists at TATRC's Biotechnology High Performance Computing Software Applications Institute (BHSAI; www.bhsai.org) have recently developed enhanced techniques to mine, systematize, and predict adverse drug-combination effects based on information in extensive databases of patient-reported events.

Sponsored by the U.S. Army's Network Science Initiative and the Defense Threat Reduction Agency (DTRA), the BHSAI focuses on developing computational models and solutions that address human health. The BHSAI team developed a methodology to predict thousands of adverse health effects based on millions of patient-reported events

combined with databases containing macromolecular drug interactions. These studies showed that roughly 10% of all drug combinations have the potential to cause an adverse effect. The results for individual drugs, drug combinations, and adverse health effects are available via AVOID (Adverse effects Of Interacting Drugs)—a searchable web-accessible database. The system has been used hundreds of times worldwide since its release in the summer of 2017.

Dr. Sven Wallqvist, Senior Research Scientist at the BHSAI, commented that “One of our main challenges as scientists today is how to make use of all the medical and chemical data that is already out there. Here, we combined data from millions of public health records with millions of drug-protein interaction data to build prediction models for thousands of adverse effects. The key to making progress is the ability to manipulate, combine, and use these data sources to make knowledge products that are easily accessible on desktops, tablets, and smartphones.” A description of this effort was recently published in *BMC Pharmacology and Toxicology*¹.

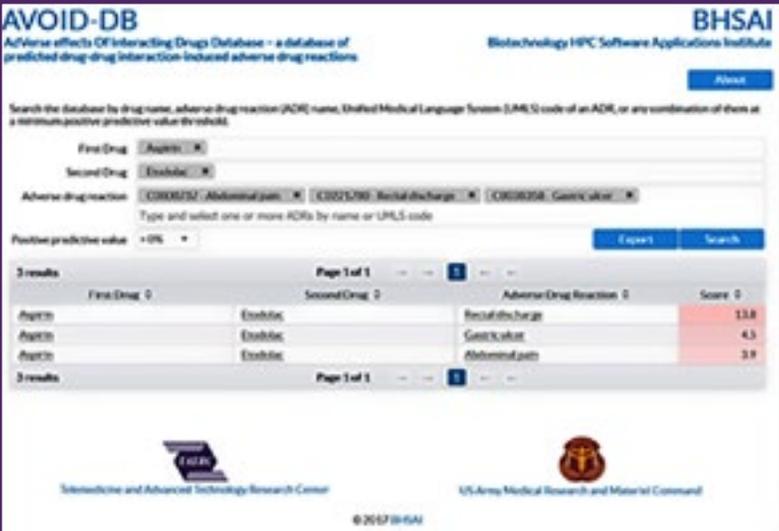
The system, which contains prediction data for approximately 800 FDA-approved drugs and their combinations, can be searched using commonly used drug names and/or ailments. The web-page can be publically accessed at <http://avoid-db.bhsai.org>.

References:

¹Liu R, AbdulHameed MDM, Kumar K, Yu X, Wallqvist A, Reifman J. Data-Driven Prediction of Adverse Drug Reactions Induced by Drug-Drug Interactions. *BMC Pharmacol Toxicol.* 2017; 18(1):44. DOI: 10.1186/s40360-017-0153-6. 



Dr. Sven Wallqvist is BHSAI's Senior Researcher leading this effort.



The screenshot shows the AVOID-DB search interface. It includes a search bar with fields for 'First Drug', 'Second Drug', and 'Adverse Drug Reaction'. Below the search bar, there are three search results displayed in a table format. The table has columns for 'First Drug 1', 'Second Drug 2', 'Adverse Drug Reaction 3', and 'Score 4'. The results are as follows:

First Drug 1	Second Drug 2	Adverse Drug Reaction 3	Score 4
Aspirin	Ethnic	Rectal discharge	13.8
Aspirin	Ethnic	Gastrocolic	4.3
Aspirin	Ethnic	Abdominal pain	3.9

At the bottom of the screenshot, there are logos for the Biotechnology High Performance Computing Software Applications Institute (BHSAI) and the U.S. Army Medical Research and Materiel Command, along with the copyright notice © 2017 BHSAI.

A screenshot of the Adverse effects Of Interacting Drugs (AVOID) database, which is publically accessible at <http://avoid-db.bhsai.org>.