Software to accurately show the adverse effects of a drug

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The computer model uses "similarity ensemble approach" (SEA), to detect similarities between the chemical drugs of the compounds and the molecules that cause side effects

A research Organization has developed a set of computer models that can predict negative side effects associated with existing drugs, By speeding up the process and increasing accuracy, the software could potentially save billions in research and decrease the number of animals used in toxicity tests. The model uses the similarities between the shape of each drug and thousands of other compounds to predict possible side effects. The theory behind the technology is that proteins can be related by their pharmacology, and these network relationships can be explored to discover new targets for established drugs.

The team ran a computer screen on 656 drugs that are already on the market, with known side effects and benefits, to predict which ones were most likely to bind to the 73 target proteins for testing drugs for side effects such as heart attacks. Then those targets were related to known side effects through a statistical method. The computer model identified 1,241 possible side-effect targets for the 656 drugs. Of the total, 348 were already in database of drug interactions while another 151 hits revealed new side effects which were later confirmed in lab testing.

"The model isn't intended to replace existing safety approaches, like lab testing and animal models, but rather as a way to prioritize very early on what sorts of lab tests must be run or which research compounds might require fewer such tests than others,"

With the computer model, it becomes possible to construct a preliminary "virtual safety panel" for almost any drugs or preclinical compound. "You'd run your drug, or even your ten thousand compounds from which one or two might someday become drugs, and ask whether any undesirable side effects 'light up' against that panel,"

Current scientific standards cannot predict how drugs will behave in relation to the targets linked to the side effects of medicines used clinically. Often, they hit more than 10 percent of the targets and the side effect targets are unrelated to previously known ones.

Finally, an impartial analysis done by a 3rd-party research group also found the software's performance to be quite promising when compared to direct bioassay.

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