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New Way To Predict Drug Side Effects

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Predicting the side-effects of a drug is not simple task. The human body has more than 1,500 molecules that are known to be involved in various diseases, and often a drug designed to hit one of these targets will also hit others that have similar structures, causing unintended consequences.

Now a group of researchers have developed a tool that can help predict the side effects of a drug by looking at all the potential interactions it might have in the human body. This tool revealed that one side effect of the AIDS drug rescriptor causes severe rashes by inadvertently targeting a hormone receptor known as histamine H4.

The scientists also found that the antidepressant drugs Prozac and Paxil were similar to beta blockers, which are used to treat hypertension -- perhaps explaining some of the shared side-effects between these different classes of drugs.

Overall, the team led by Bryan Roth at the University of North Carolina at Chapel Hill and Brian Shoichet at the University of California, San Francisco predicted some 1,800 new "off-target" associations. They tested a number of these experimentally and confirmed 23 of them, reported in the scientific journal *Nature*.

They uncovered these interactions by comparing 3,665 existing and experimental drugs with more than 65,000 chemicals that are known to bind to hundreds of human proteins. Strong similarities between the drugs and any of the 65,000 chemicals predicted that both might bind to the same proteins.

Besides making it easier to screen for drug toxicities, said Shoichet, the method may make it possible to look for additional targets of existing drugs.

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