New method uncovers side effects before a drug hits the market

Side effects are a major reason that drugs are taken off the market and a major reason why patients stop taking their medications, but scientists are now reporting the development of a new way to predict those adverse reactions ahead of time. The report on the method, which could save patients from severe side effects and save drug companies time and money, appears in ACS' *Journal of Chemical Information and Modeling*.

Yoshihiro Yamanishi and colleagues explain that drug side effects are a major health problem—the fourth-leading cause of death in the U.S.—which by some estimates claim 100,000 lives every year. Serious side effects are the main reason why existing drugs must be removed from the market and why pharmaceutical companies halt development of new drugs after investing millions of dollars. Current methods of testing for side effects are costly and inaccurate. That's why the scientists sought to develop a new computer-based approach to predicting possible side effects.

They show the usefulness of their proposed method on simultaneous prediction of 969 side effects of 658 drugs that already are in wide medical use. The method is based on knowledge about chemical and biological information about ingredients in these medications. They also used the approach to identify possible side effects for many uncharacterized molecules. Based on that work, the scientists conclude that the new method could be helpful in uncovering serious side effects early in the development and testing of new drugs, avoiding costly investment in medications unsuitable for marketing.

Drug Side-Effect Prediction Based on the Integration of Chemical and Biological Spaces [1]

Source: American Chemical Society [2]

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