Researchers develop more computer-aided drug design

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Researchers in Germany report an advance toward the much awaited era in which scientists will discover and design drugs for cancer, arthritis, AIDS and other diseases almost entirely on the computer, instead of relying on the trial-and-error methods of the past. Their study is scheduled for the March 24 issue of ACS' *Journal of Chemical Information and Modeling*.

In the report, Michael C. Hutter and colleagues note that computer-aided drug design already is an important research tool. The method involves using computers to analyze the chemical structures of potential drugs and pinpoint the most promising candidates.

Existing computer programs check a wide range of chemical features to help distinguish between drug-like and nondrug materials. These programs usually cannot screen for all features at the same time, an approach that risks overlooking promising drug-like substances.

In the new study, researchers describe a more gradual and efficient system. Their new program uses an initial quick screen for drug-like features followed immediately by a second, more detailed screen to identify additional drug-like features. They applied this new classification scheme to a group of about 5,000 molecules that had previously been screened for drug-like activity. The new strategy was more efficient at identifying drug-like molecules "whereby up to 92 percent of the nondrugs can be sorted out without losing considerably more drugs in the succeeding steps," the researchers say.

Source: ACS