

New drugs awaiting discovery in Chinese herbs?

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The first large-scale computer screenings of Chinese herbs -- commonly used in traditional Chinese medicine -- has revealed a wide variety of compounds with potential for use in treating HIV/AIDS, cancer, Alzheimer's Disease, arthritis and other diseases, according to scientists in London.

In an article scheduled for the March 26 issue of the ACS' *Journal of Chemical Information and Modeling*, a bi-monthly publication, David J. Barlow and colleagues note that such in silico research is becoming increasingly effective in identifying promising compounds that could be candidates for drug development.

In silico ("in silicon") means research done on computers or via computer simulation and has joined the in vivo and in vitro experiments traditionally used in the life sciences.

The researchers screened a database of chemical structures of Chinese herbal constituents from 240 species of plants for possible activity against various diseases.

About 62 percent of the species were found to contain chemicals with characteristics required for activity against at least one disease and 53 percent against two or more diseases. The study also describes corroborative evidence from the scientific literature that supported many of the computer predictions. In a companion article in the journal, the researchers describe the herbal databases.



Source: American Chemical Society

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