Predicting serious drug side effects before they occur

March 28 2011

All medications have side-effects from common aspirin to herbal remedies and from standard anticancer drugs to experimental immunosuppressants. However, predicting important side effects, serious adverse drug reactions, ADRs, is with current understanding almost impossible. However, a neural network technology trained with past data could give drug companies and healthcare workers a new tool to spot the potential for ADRs with any given medication.

Writing in the *International Journal of Medical Engineering and Informatics*, at team from the University of Medicine and Dentistry of New Jersey, has developed a new model that tests show is 99.87 percent accurate in predicting adverse drug reactions among 10,000 observations and 100 percent for non-serious ADRs.

Peng-fang Yen and colleagues Dinesh Mital and Shankar Srinivasan explain how obligatory warning labels on medication packaging often serve only to cause concern among patients, while products withdrawn from the market because of repeated ADRs repeatedly undermine the pharmaceutical industry. From the medical industry's point of view and the perspective of patients, this is a growing concern that might be remedied with new technology, saving lives, reputations and healthcare costs.

The Food Drug Administration (FDA) in USA and the World Health Organization (WHO) monitor the safety of medications continuously. However, technology that could identify possible ADRs at the earliest

possible stage of drug development, licensing and marketing is urgently needed, especially given the potential risks to patients in emerging areas of healthcare and the potential risks to shareholder confidence.

The team's artificial neural network is a mathematical model of the biologic neural network embedded in computer software. It is trained by feeding in structural and physical data associated with known pharmaceutical products and any ADRs. A feedback loop discards those connections where a wrong prediction of a known outcome is made and as data are added the ANN builds up a network of correct "predictions". After sufficient training, the ANN can then be tested on another set of pharmaceuticals and outcomes checked against known ADRs. If confidence is sufficiently high, the ANN can be used to predict ADRs for new drugs.

The team has demonstrated an accuracy of 95 percent in preliminary tests and is now using a much larger data set of 10,000 drug molecules and ADR observations to train the ANN to a much more refined level.

More information: "Prediction of the serious adverse drug reactions using an artificial neural network model" in Int. J. Med. Eng. Informat., 2011, 3, 53-59

Provided by Inderscience Publishers