Data Analysis

CNIO Launches Online Tool to Extract Drug Toxicity Information from Text

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The Biological Text Mining Unit presents in a recent *Nucleic Acids Research* paper the LimTox online software tool developed at the Spanish National Cancer Research Centre (CNIO). This resource integrates state-of-the-art in text mining, machine learning and language technology methods in order to empower the underlying biomedical semantic search engine. LimTox allows retrieval and ranking of chemical and biological entities of interest, interactions between them, visualization of chemical structures of compound mentions detected

automatically in running text and generation of entity relation network graphs.

There is an increasing interest in more sophisticated search engines that are tailored to cope with the complexity of biomedical data, not only enabling more targeted search queries but also easier integration and construction of biological knowledgebases and analysis of experimental datasets.

"There has already been some substantial work on text mining of genes, but far less on chemicals", explains Martin Krallinger, head of the Biological Text Mining Unit and main author of the paper. "To address this limitation -he ads-, we have implemented this system".

A systematic strategy for efficient online access to both biological and chemical information contained in scientific literature and medical agency reports is critical for scientific intelligence and the subsequent decision-making in areas such as chemical-biology, drug discovery, toxicology and pharmacogenetics.

LimTox has a special focus on adverse reactions and chemical compound toxicity with emphasis on drug-induced liver injury, including substances that cause worsening of hepatic function and hepatocarcinogenesis. It also enables systematic access of relevant information related to other adverse reactions (nephrotoxicity, cardiotoxicity, thyrotoxicity, phospholipidosis), alteration of biochemical liver markers and key enzymes for drug metabolism (P450 cytochromes -CYPs).

"Among the potential candidate toxicological end points hepatotoxicity represents one of the most critical toxic effects at the organ level. The liver is a fundamental organ examined in toxicology studies, due to its central role in metabolic, excretory and synthetic biochemical pathways, and the mechanisms leading to drug-induced liver toxicity are particularly complicated", sais Krallinger.

The online-based tool provides information on drug hepatotoxicity extracted from abstracts and full text papers from the biomedical archive PubMed, the European Public Assessment Reports (EPAR), published by the European Medicines Agency (EMA), and the United States New Drug Application (NDA).
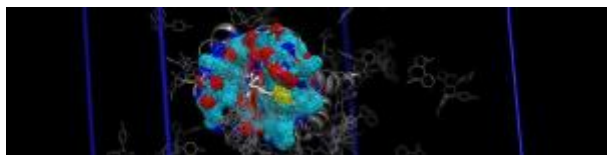
The LimTox webserver can help researchers and clinicians to retrieve more efficiently associations to adverse reactions by using both, simple

keyword searches as well as queries particularly optimized to handle
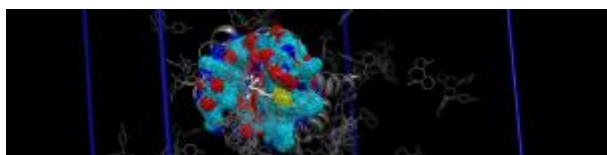entities such as chemicals and genes.

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