In silico prediction of gene expression profiles for drug-like compounds based on their structural formulae

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Drug-induced gene expression profile is a major determinant of drug action on cell. Experimentally determined profiles are used to solve different problems in drug development and clinical practice such as drug repositioning and resistance, toxicity and drug-drug interactions (DDI). The information about drugs' influence on gene expression is freely available from the Comparative Toxicogenomics Database (http://ctdbase.org/). We used this data for training and validation of computer system to perform qualitative prediction of gene expression profiles of drugs based on their structural formulae. SAR models were created using PASS software that we develop and update for about 20 years (http://www.pharmaexpert.ru/PASSOnline). A freely available web-service for prediction of drug-induced gene expression profiles has been developed (http://www.pharmaexpert.ru/GE). Predicted gene expression profiles can be used for analysis of drug resistance, drug synergistic effects and DDI. The work was partially supported by RFBR/NIH grant No 12-04-91445-NIH_A/RUB1-31081-MO-12, and RFBR grant No 12-07-00597-a.