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A Computational Study Concerning the Biological Effects of the Most Commonly Used Phthalates

Authors : Dana Craciun, Daniela Dascalu, Adriana Isvoran

Abstract : Phthalates are a class of plastic additives that are used to enhance the physical properties of plastics and as solvents in paintings and some of them proved to be of particular concern for the human health. There are insufficient data concerning the health risks of phthalates and further research on evaluating their effects in humans is needed. As humans are not volunteers for such experiments, computational analysis may be used to predict the biological effects of phthalates in humans. Within this study we have used some computational approaches (SwissADME, admetSAR, FAFDrugs) for predicting the absorption, distribution, metabolization, excretion and toxicity (ADME-Tox) profiles and pharmacokinetics for the most common used phthalates. These computational tools are based on quantitative structure-activity relationship modeling approach. The predictions are further compared to the known effects of each considered phthalate in humans and correlations between computational results and experimental data are discussed. Our data revealed that phthalates are a class of compounds reflecting high toxicity both when ingested and when inhaled, but by inhalation their toxicity is even greater. The predicted harmful effects of phthalates are: toxicity and irritations of the respiratory and gastrointestinal tracts, dyspnea, skin and eye irritations and disruption of the functions of liver and of the reproductive system. Many of investigated phthalates are predicted to be able to inhibit some of the cytochromes involved in the metabolism of numerous drugs and consequently to affect the efficiency of administrated treatments for many diseases and to intensify the adverse drugs reactions. The obtained predictions are in good agreement with clinical data concerning the observed effects of some phthalates in cases of acute exposures. Our study emphasizes the possible health effects of numerous phthalates and underlines the applicability of computational methods for predicting the biological effects of xenobiotics.

Keywords : phthalates, ADME-Tox, pharmacokinetics, biological effects
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