Computational Toxicology: Chapter 5. Integrated Systems Biology Approaches to Predicting Drug-Induced Liver Toxicity: A Dynamic Systems Model of Rat Liver ... Measurements to Predict In Vivo Toxicity

Kalyanasundaram Subramanian

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Liver injury is the most common cause of post-marketing drug withdrawal. Predicting toxicity observed in the clinic, especially idiosyncratic toxicity, is extremely challenging. In this chapter we developed a predictive system that integrates different data types and provides insight into the mechanisms of drug-induced liver injury. This is a dynamic systems approach based on the mathematical modeling of the kinetics of metabolic pathways involved in liver homeostasis. Drug-induced perturbations to this homeostasis that lead to toxicity can be measured by targeted in vitro assays. Several physiological and pathological situations can be accurately modeled by integrating in silico and in vitro methods. What we also demonstrate is that the method is flexible enough to allow an understanding of the mechanistic basis for idiosyncratic toxicity and individual variations in toxic responses. It can also be used along with functional genomic data to generate mechanistic hypotheses of drug action.

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