Computational Toxicology: Chapter 10. Computational Toxicology Experience and Applications for Risk Assessment in the Pharmaceutical Industry

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The costs of developing new drugs continue to rise while public and governmental expectations demand safer drugs. This demand for safer drugs can also significantly delay the time it takes to reach the market, as screening for drug safety can be a time-consuming process. In order to reduce costs and timelines while increasing safety, pharmaceutical firms have incorporated predictive methodologies to identify potential safety issues before a new drug is given to patients or even before a compound is tested in animals. Initial predictive efforts have focused on using compound structure to predict toxicity. This work has led to a number of successes in the ability to predict genotoxicity and carcinogenicity. In this chapter, we describe some of the methods used in pharmaceuticals to predict these adverse effects as well as methodologies used to predict organ-specific toxicity such as drug-induced liver injury, a major risk for new drugs. More recently, pharmaceuticals have begun to consider gene information when predicting toxicities. Activity against major risk genes such as the hERG is now routinely used to identify some risks. Finally, we discuss some approaches being developed to predict and/or categorize risk using gene, protein, or metabolite changes.

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