



## **TOXICITY PATHWAYS AND MODELS: MINING FOR POTENTIAL OFF-TARGET EFFECTS**

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In recent years there has been considerable research into developing better in silico, in vitro and in vivo methods and models for toxicology. This is desirable, as the pharmaceutical industry needs to prospectively identify molecules as early as possible that might fail in the clinic due to toxicity. Computational technologies can be used to mine the biological and chemistry knowledge that may be relevant to toxicology. For example they could be used to analyze in vitro gene expression data and develop gene signatures for hepatotoxicity or other toxicities. Databases can also be used to leverage the power of cheminformatics and use the plethora of methods developed in this area to deal with toxicity information. Several examples of such databases and applications will be discussed. A key issue is the seamless integration of all available data. A global understanding of toxic effects may ultimately lead to the development of safer drugs.