Joint Topical Collection
Predictive Toxicology

Message from the Collection Editor

The recent advances of toxicogenomics, high-throughput screening, stem cells, and image analysis are creating unique opportunities to improve our ability to predict risk in humans and the development of predictive toxicology. These modern biotechnologies are producing big toxicological data and require advanced artificial intelligence technologies to evaluate the potential for predicting toxicity. The application of conventional machine learning algorithms, such as logical regression, decision tree, and support vector machines, have largely enhanced our capability to recover useful knowledge from the increasing volume of toxicity data. A recent study reported by researchers from John Hopkins University, demonstrated that using artificial intelligent algorithms trained on chemical-safety, big data could be more predictive and outperform expensive animals studies on some toxicities. In this Topical Collection, we focus on exploring the relationship between the toxicity of xenobiotics and their chemical structures, disturbed cellular, and molecular pathways by the application of artificial intelligent methods to improve the prediction of toxicity risk.

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