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化学構造情報とインビトロ試験を活用した化学物質の安全性評価手法の開発：薬物代謝を考慮した評価系の重要性

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Development of Chemical Safety Evaluation System Using Chemical Structural Information and *in vitro* Testing: Importance of a Drug Metabolism-Integrated System

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Abstract

Currently, the toxicity evaluation of chemical substances is conducted mainly based on the results of animal experiments, but from the viewpoint of animal welfare and development efficiency, the development of alternatives to animal experiments is highly required. To this end, many studies are conducted to understand the toxicity mechanism and to construct *in vitro* testing systems based on the mechanism. In addition, due to its high throughput, the development of an *in silico* method using machine learning technics with chemical structure information as alternatives to animal experiments is also attracting great attention from researchers. Since the toxicity of some chemical substances is caused by their metabolites, the development of *in vitro* and *in silico* evaluation systems that consider drug metabolism is also required. However, current toxicity evaluation systems do not necessarily consider drug metabolism. In this article, I will introduce our recent findings on the importance of drug metabolism consideration in chemical toxicity evaluation using *in vitro* and *in silico* methods.

Key words:　Toxicity prediction, Drug metabolism, Molecular descriptor, *In vitro* testing, Decision tree.