Development of the Discriminant KY-methods for Toxicity Screening

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The KY-methods are powerful data analysis methods which enables a perfect classification even if overlapping between classes of samples is very high and number of samples is quite large.

KY-methods have been developed on the premise that applied on toxicity prediction research field. The special features of the KY-methods are as follows. This approach can overcome various difficult data analysis conditions.

These are conditions which make extremely difficult to do a data analysis. For example, number of sample is very large, the spread of the sample space is large because structure diversity of compounds is quite large, and more overlapping between classes in the sample space is large.

On the toxicity prediction research fields, it have been almost impossible to achieve high classification value by simple application of multivariate analysis / pattern recognition methods by conventional approaches.

Basics of the KY-methods are the multi-step operations that repeat classification and sample re-construction.

Currently, three different discriminant analysis methods have been developed in accordance with the basics of the KY-methods. In this report, briefly discuss the current development status of the KY-methods.

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